



## wwPDB EM Validation Summary Report ⓘ

Nov 3, 2024 – 08:58 pm GMT

PDB ID : 7PAL  
EMDB ID : EMD-13276  
Title : 70S ribosome with A- and P-site tRNAs in Mycoplasma pneumoniae cells  
Authors : Xue, L.; Lenz, S.; Rappsilber, J.; Mahamid, J.  
Deposited on : 2021-07-30  
Resolution : 4.70 Å(reported)  
Based on initial models : 7OOD, 7OOC, 4V7C, 3J9W

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

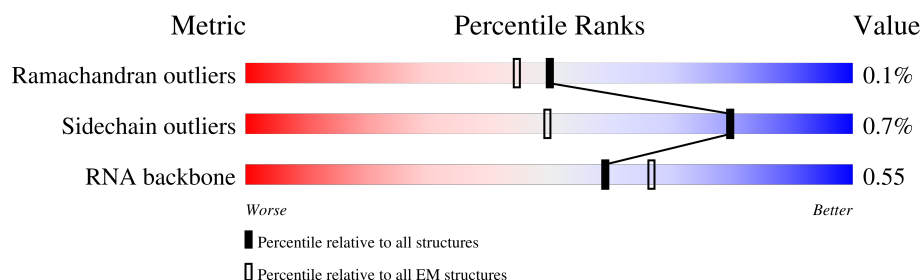
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	48	
2	1	59	
3	2	37	
4	A	294	
5	B	273	
6	C	205	
7	D	219	
8	E	215	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	F	155	43% 99%
10	G	142	25% 99%
11	H	132	36% 96%
12	I	108	34% 94%
13	J	121	24% 94%
14	K	139	15% 96%
15	L	124	49% 95%
16	M	61	13% 98%
17	N	86	23% 97%
18	O	94	26% 83%
19	P	85	32% 98%
20	Q	104	17% 62%
21	R	87	40% 95%
22	S	87	17% 85%
23	T	60	25% 88%
24	Z	5	100%
25	a	287	7% 99%
26	b	287	6% 80%
27	c	212	13% 99%
28	d	180	49% 96%
29	e	184	27% 95%
30	f	149	83% 96%
31	g	161	64% 70%
32	h	137	87% 93%
33	i	146	11% 98%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	j	122	
35	k	151	
36	l	139	
37	m	124	
38	n	116	
39	o	119	
40	p	127	
41	q	100	
42	r	159	
43	s	237	
44	t	111	
45	u	104	
46	v	65	
47	w	111	
48	x	97	
49	y	57	
50	z	53	
51	3	2907	
52	4	108	
53	5	1520	
54	6	76	
54	7	76	
55	Y	9	

## 2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 146334 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	47	Total	C	N	O	S	0	0
			380	236	81	61	2		

- Molecule 2 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	59	Total	C	N	O	S	0	0
			477	300	99	77	1		

- Molecule 3 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	37	Total	C	N	O	S	0	0
			304	189	65	46	4		

- Molecule 4 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	240	Total	C	N	O	S	0	0
			1921	1226	334	352	9		

- Molecule 5 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	215	Total	C	N	O	S	0	0
			1698	1073	313	307	5		

- Molecule 6 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	203	Total	C	N	O	S	0	0
			1660	1051	314	290	5		

- Molecule 7 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	153	Total	C	N	O	S	0	0
			1173	742	226	202	3		

- Molecule 8 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	167	Total	C	N	O	S	0	0
			1362	857	240	263	2		

- Molecule 9 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	154	Total	C	N	O	S	0	0
			1246	785	239	216	6		

- Molecule 10 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	141	Total	C	N	O	S	0	0
			1110	723	193	192	2		

- Molecule 11 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	128	Total	C	N	O	S	0	0
			1028	655	191	181	1		

- Molecule 12 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	101	Total	C	N	O	S	0	0
			809	523	142	143	1		

- Molecule 13 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	114	Total	C	N	O	S	0	0
			829	514	153	156	6		

- Molecule 14 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	136	Total	C	N	O	S	0	0
			1076	680	213	181	2		

- Molecule 15 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	118	Total	C	N	O		0	0
			951	594	191	166			

- Molecule 16 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	60	Total	C	N	O	S	0	0
			474	302	96	72	4		

- Molecule 17 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	83	Total	C	N	O		0	0
			673	428	125	120			

- Molecule 18 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	80	Total	C	N	O	S	0	0
			646	414	119	111	2		

- Molecule 19 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	83	Total	C	N	O		0	0
			675	425	135	115			

- Molecule 20 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	65	Total	C	N	O	S	0	0
			535	342	103	86	4		

- Molecule 21 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	84	Total	C	N	O	S	0	0
			682	435	127	118	2		

- Molecule 22 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	77	Total	C	N	O	S	0	0
			629	383	135	111			

- Molecule 23 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	T	53	Total	C	N	O	S	0	0
			471	295	103	72	1		

- Molecule 24 is a protein called nascent peptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	5	Total	C	N	O	S	0	0
			31	20	5	6			

- Molecule 25 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	285	Total	C	N	O	S	0	0
			2225	1385	437	397	6		

- Molecule 26 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	229	Total	C	N	O	S	0	0
			1762	1119	318	318	7		

- Molecule 27 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	210	Total	C	N	O	S	0	0
			1644	1047	297	297	3		

- Molecule 28 is a protein called 50S ribosomal protein L5.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	175	Total	C	N	O	S	0	0
			1388	893	245	246	4		

- Molecule 29 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	e	176	Total	C	N	O	S	0	0
			1396	899	247	250			

- Molecule 30 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	f	145	Total	C	N	O	S	0	0
			1160	746	204	207	3		

- Molecule 31 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	g	126	Total	C	N	O	S	0	0
			960	612	167	178	3		

- Molecule 32 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	h	128	Total	C	N	O	S	0	0
			959	616	160	177	6		

- Molecule 33 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	i	144	Total	C	N	O	S	0	0
			1164	737	213	209	5		

- Molecule 34 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	j	122	Total	C	N	O	S	0	0
			944	595	178	167	4		

- Molecule 35 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	k	148	Total	C	N	O		
			1153	731	226	196	0	0

- Molecule 36 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	l	136	Total	C	N	O	S		
			1079	694	196	182	7	0	0

- Molecule 37 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	m	119	Total	C	N	O	S		
			958	609	175	171	3	0	0

- Molecule 38 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	n	112	Total	C	N	O	S		
			889	557	175	155	2	0	0

- Molecule 39 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	o	115	Total	C	N	O	S		
			938	592	180	165	1	0	0

- Molecule 40 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	p	114	Total	C	N	O	S		
			947	603	188	154	2	0	0

- Molecule 41 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	q	99	Total	C	N	O	S		
			811	525	148	134	4	0	0

- Molecule 42 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	r	139	Total	C	N	O	S	0	0
			1068	663	207	191	7		

- Molecule 43 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	s	92	Total	C	N	O	S	0	0
			720	475	122	122	1		

- Molecule 44 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	t	111	Total	C	N	O	S	0	0
			872	550	166	153	3		

- Molecule 45 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	u	86	Total	C	N	O	S	0	0
			657	409	130	117	1		

- Molecule 46 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	v	63	Total	C	N	O	S	0	0
			513	317	108	87	1		

- Molecule 47 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	w	100	Total	C	N	O	S	0	0
			818	517	153	148			

- Molecule 48 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	x	44	Total	C	N	O	S	0	0
			344	221	55	64	4		

- Molecule 49 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	y	56	Total	C	N	O	S	0	0
			452	274	98	75	5		

- Molecule 50 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	z	50	Total	C	N	O	S	0	0
			408	255	81	68	4		

- Molecule 51 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	3	2878	Total	C	N	O	P	0	0
			61664	27558	11236	19995	2875		

- Molecule 52 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	4	105	Total	C	N	O	P	0	0
			2239	1003	409	724	103		

- Molecule 53 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	5	1493	Total	C	N	O	P	0	0
			31943	14279	5792	10382	1490		

- Molecule 54 is a RNA chain called tRNA-Phe.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	6	76	Total	C	N	O	P	0	0
			1618	723	289	531	75		
54	7	76	Total	C	N	O	P	0	0
			1618	723	289	531	75		

- Molecule 55 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Y	9	Total	C	N	O	P	0	0
			183	84	29	62	8		

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

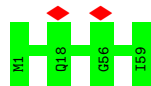
- Molecule 1: 50S ribosomal protein L34

Chain 0:  98%



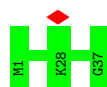
- Molecule 2: 50S ribosomal protein L35

Chain 1:  100%




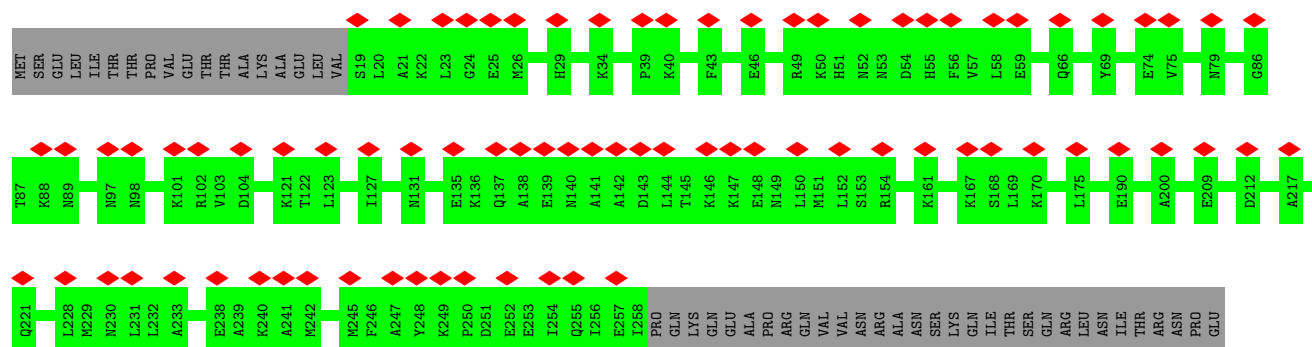
- Molecule 3: 50S ribosomal protein L36

Chain 2:  100%




- Molecule 4: 30S ribosomal protein S2

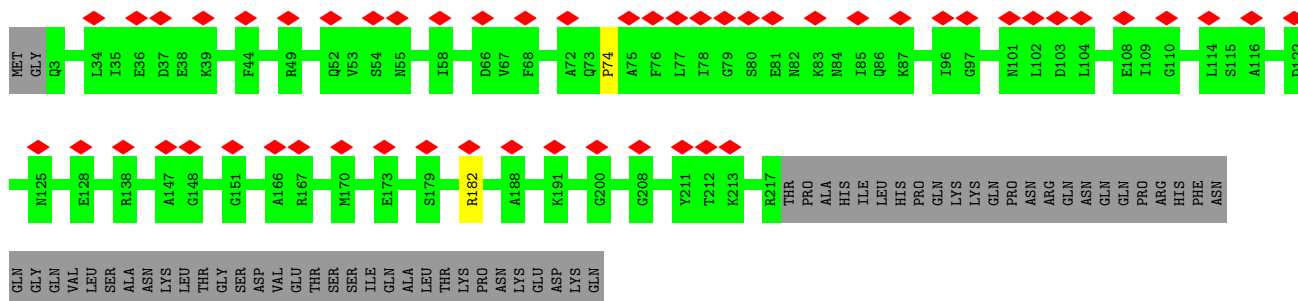
Chain A:  27% 82% 18%



VAL  
LEU  
THR  
ARG  
GLU

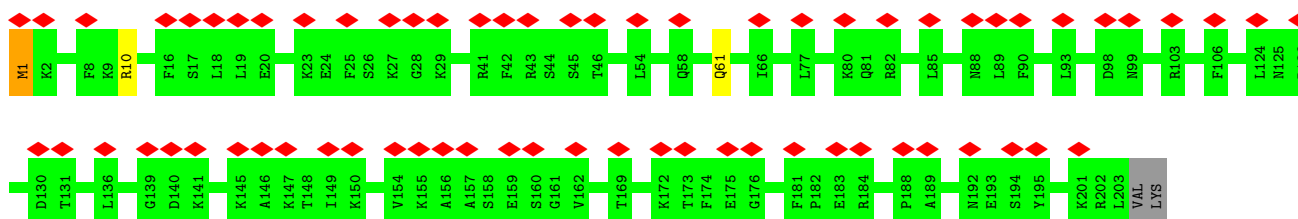
• Molecule 5: 30S ribosomal protein S3

Chain B: 



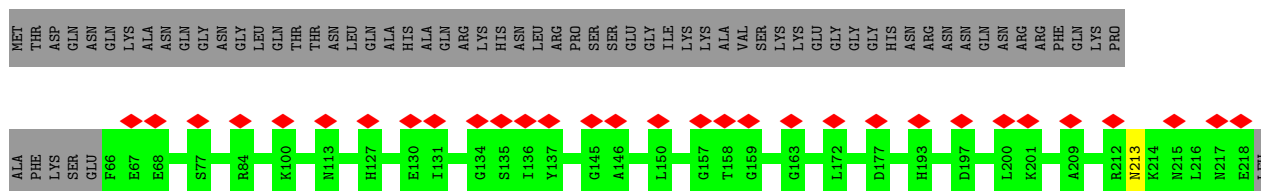
• Molecule 6: 30S ribosomal protein S4

Chain C: 




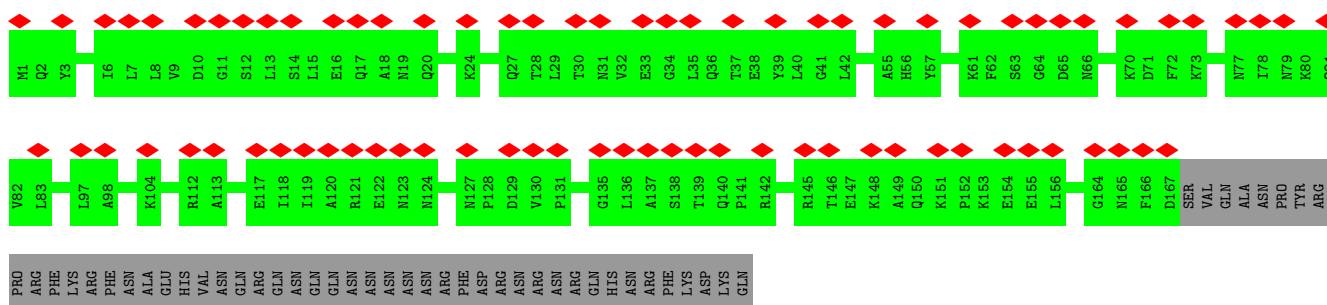
• Molecule 7: 30S ribosomal protein S5

Chain D: 

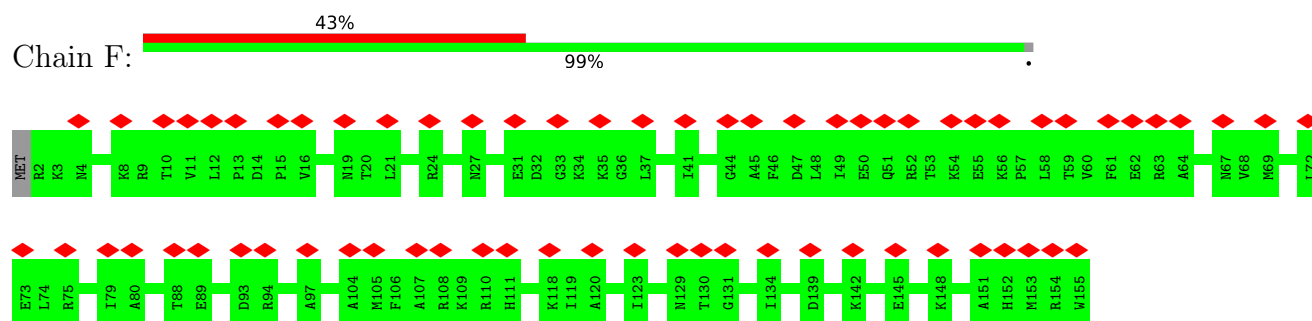


• Molecule 8: 30S ribosomal protein S6

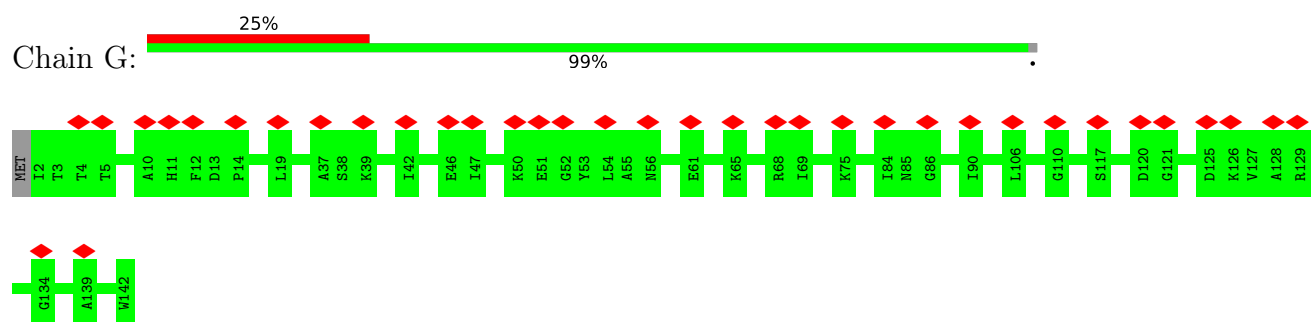
Chain E: 



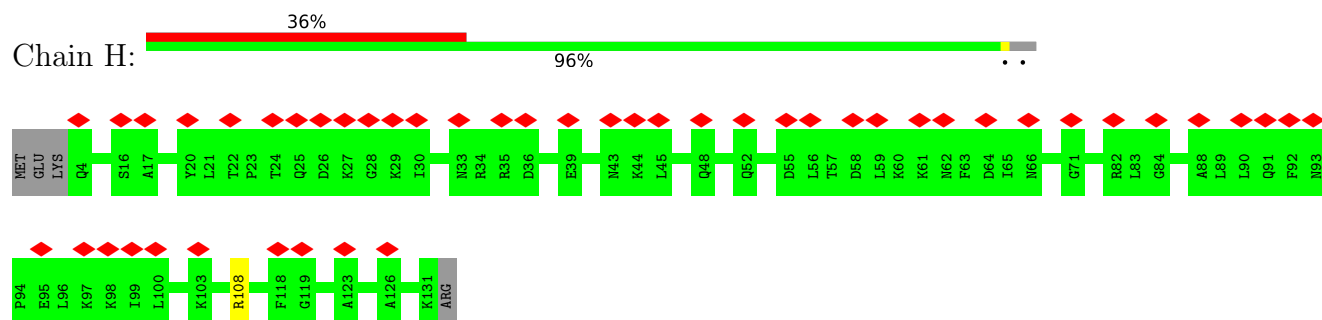
- Molecule 9: 30S ribosomal protein S7



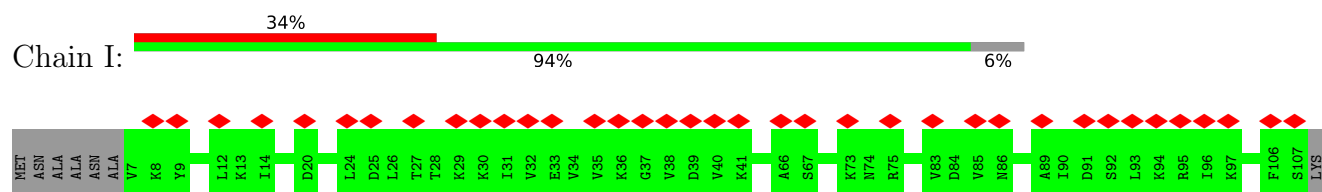
- Molecule 10: 30S ribosomal protein S8



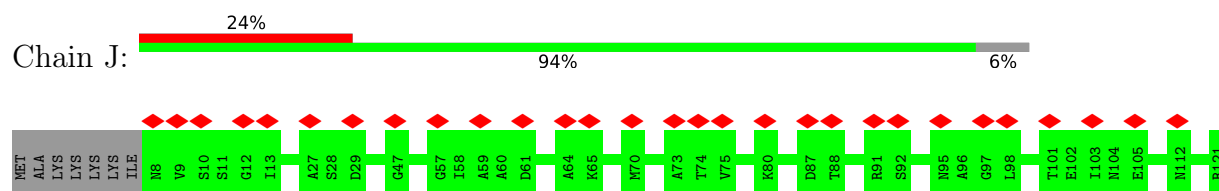
- Molecule 11: 30S ribosomal protein S9



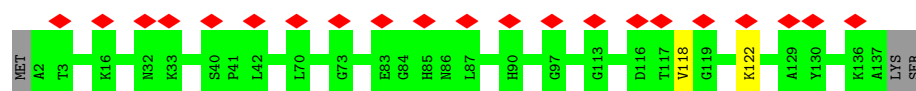
- Molecule 12: 30S ribosomal protein S10



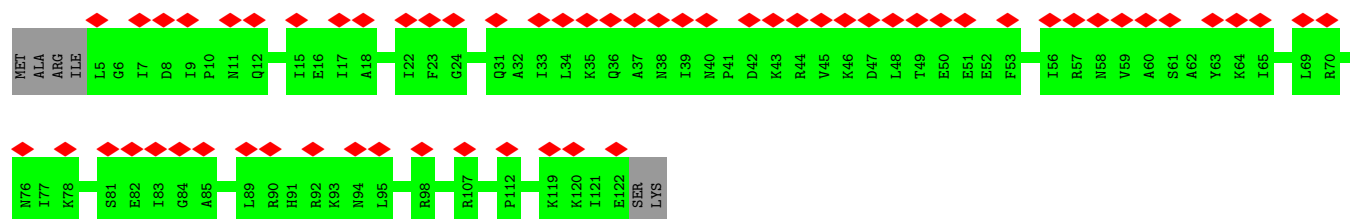
- Molecule 13: 30S ribosomal protein S11



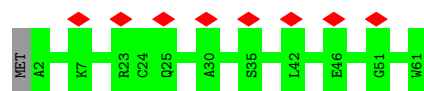
- Molecule 14: 30S ribosomal protein S12



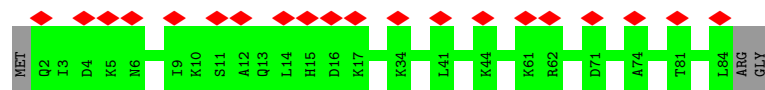
- Molecule 15: 30S ribosomal protein S13



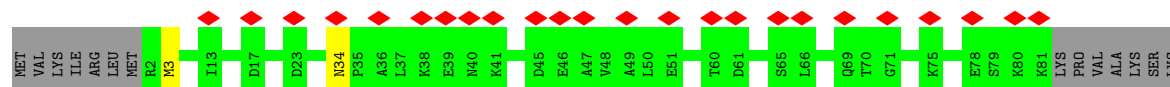
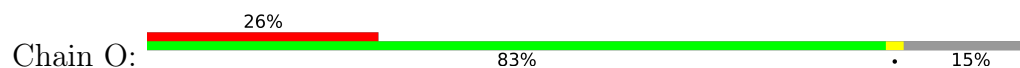
- Molecule 16: 30S ribosomal protein S14 type Z



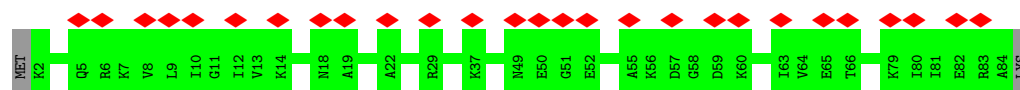
- Molecule 17: 30S ribosomal protein S15



- Molecule 18: 30S ribosomal protein S16



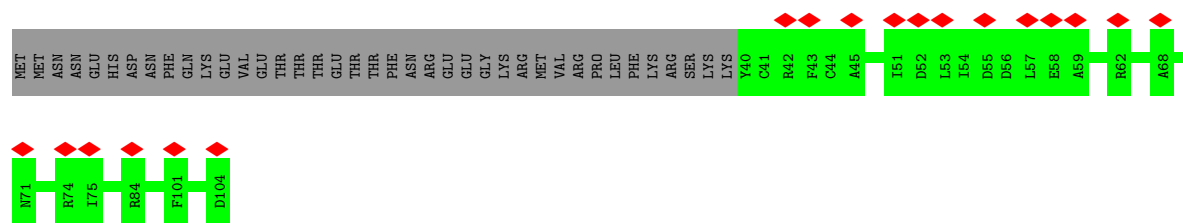
- Molecule 19: 30S ribosomal protein S17



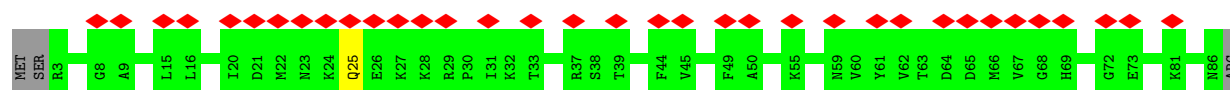
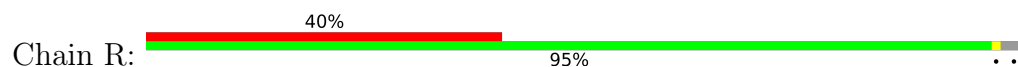
- Molecule 20: 30S ribosomal protein S18



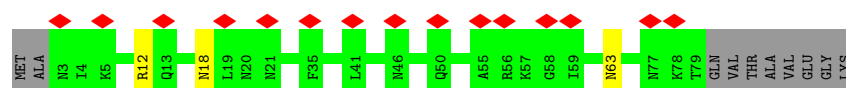
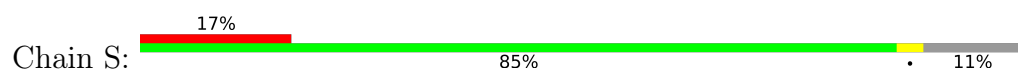




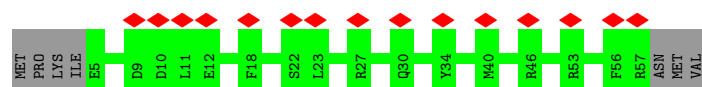
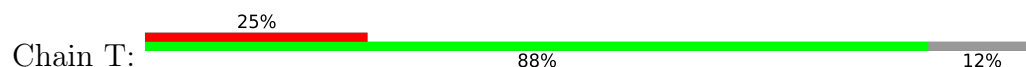
- Molecule 21: 30S ribosomal protein S19



- Molecule 22: 30S ribosomal protein S20



- Molecule 23: 30S ribosomal protein S21

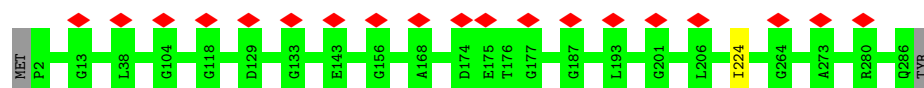


- Molecule 24: nascent peptide

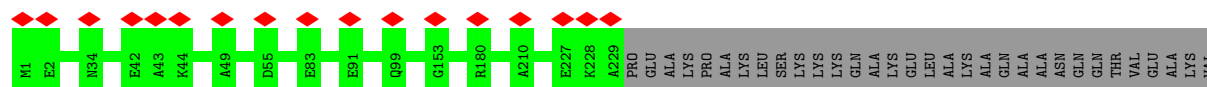
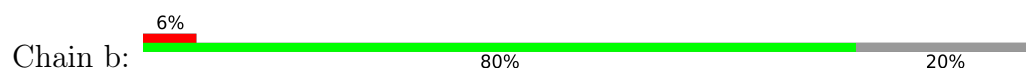


There are no outlier residues recorded for this chain.

- Molecule 25: 50S ribosomal protein L2



- Molecule 26: 50S ribosomal protein L3



ASP  
THR  
PRO  
VAL  
VAL  
GLU  
PRO  
LYS  
PRO  
THR  
GLU  
VAL  
LYS  
LYS  
ALA  
ALA  
VAL  
PRO  
VAL  
VAL  
GLU  
LYS  
LYS  
GLY  
GLY  
ASP  
LYS

• Molecule 27: 50S ribosomal protein L4

Chain c:  13% 99%

MET A2 K3 G11 S12 T15 E16 K19 G23 L24 I25 A26 K27 E28 Q42 E57 G77 L112 S122 D123 D129 L132 F133 N134 L153 D154 K155 E169 D184 N195 E200 L207 F211 LYS

• Molecule 28: 50S ribosomal protein L5

Chain d:  49% 96%

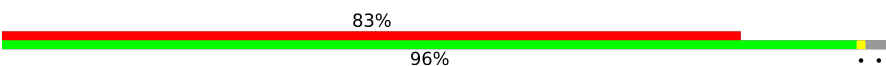
MET ASN N3 L4 K5 Y8 A13 K14 E15 K18 S19 F20 S23 Q27 E32 K38 D42 A43 I44 R45 D46 S47 K48 F49 L50 E51 S52 N55 E56 L59 I60 Q63 K69 A70 K71 N72 D144 A73 I74 S75 K78 L79 R80 A81 G82 I85 G86 C87 T90 L91 R92 G93 E94 L100 E101 K102 L103 I104 A107 R110 V111 R112 F114 R115 G116 S118 L119 K120 S121 F122 D123 G124 R125 I132 K133 E134 Q135 I136 I137 F138 P139 E140 I141 V142 Y143 D144 I145 I146 K147 R148 I149 R150 G151 F152 D153 V154 T155 L156 S159 T160 N161 K162 D163 S164 E165 A166 L169 L170 R171 A172 L173 N174 L177 VAL LYS GLY

• Molecule 29: 50S ribosomal protein L6

Chain e:  27% 95%

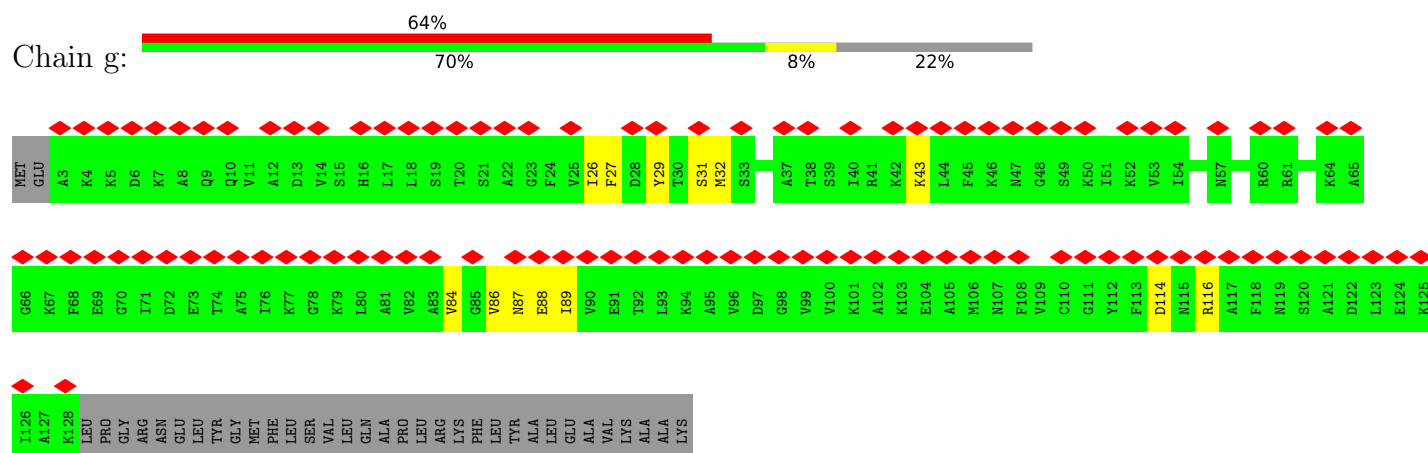
MET SER K3 I9 D12 P13 A14 K15 V16 N17 L18 N19 F20 Q21 K22 D23 V27 K28 G29 P30 L31 G32 Q33 I34 E35 L36 K37 K45 F46 E47 L48 K49 D50 N51 N52 E60 I66 I79 I80 G81 G85 F86 E87 L90 R91 E102 G103 E104 H114 K122 G123 E129 K130 N131 T132 T135 I136 S137 E150 K153 G164 V165 L166 D169 E170 V171 I172 K178 THR ALA GLY LYS LYS

• Molecule 30: 50S ribosomal protein L9

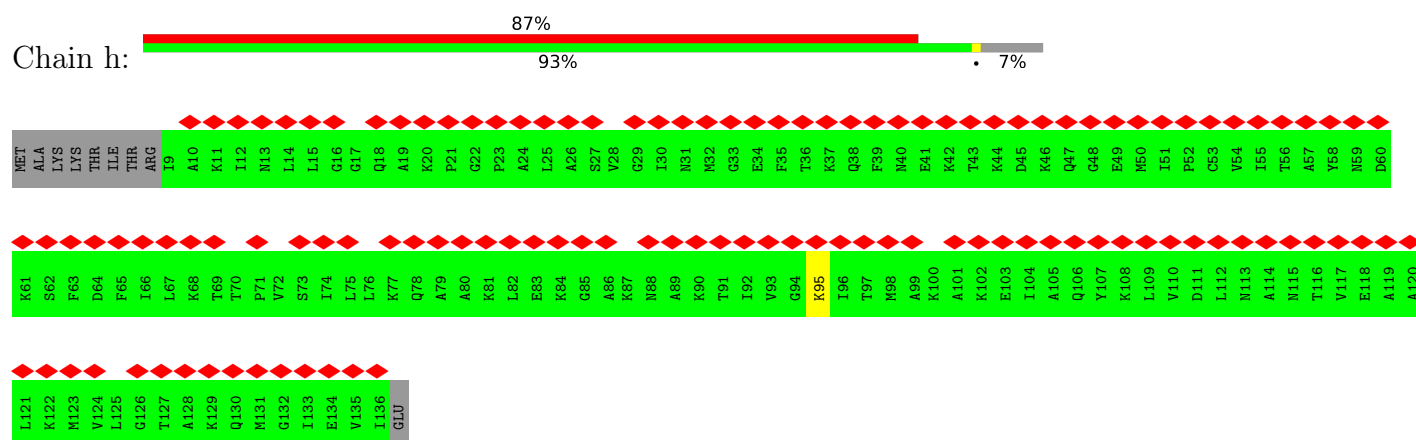
Chain f:  83% 96%

M1 K2 Q7 D8 S10 N11 G13 K14 R15 F16 D17 V18 V21 K22 Y25 A26 I27 H28 F29 P38 L39 T40 K41 K42 S43 H102 L44 Q45 D46 D47 D48 L49 F50 L51 K52 K53 Q54 Q55 E56 H57 Y58 E59 I60 N61 K62 A63 L64 S65 H66 K67 K69 E70 V71 I72 E73 Q74 T75 E76 L77 H78 F79 S80 L81 K82 E83 H84 N85 G86 R87 P88 Y89 S91 I92 I93 T94 K95 Q96 I97 I98 N99 Q100 A101 H102 T103 K104 M106 A107 L108 Q109 K110 F111 M112 F113 K114 D115 N116 V117 R118 L119 G120 F121 D122 D123 H124 E125 I126 L128 H129 I130 F131 E132 D133 T134 T135 A136 V137 L138 K139 V140 K141 V142 T143 P144 D145 ASN GLY VAL LYS

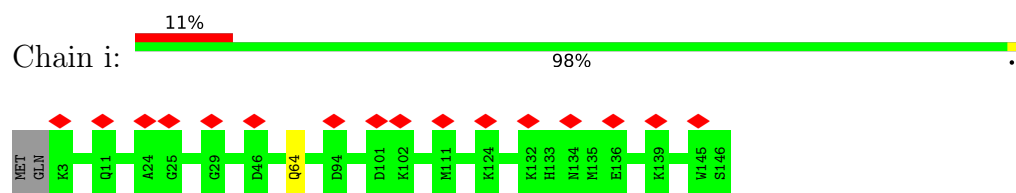
- Molecule 31: 50S ribosomal protein L10



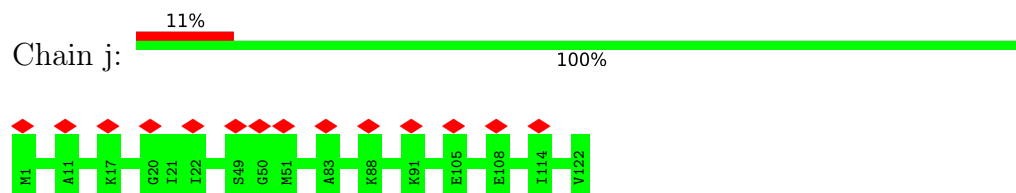
- Molecule 32: 50S ribosomal protein L11



- Molecule 33: 50S ribosomal protein L13

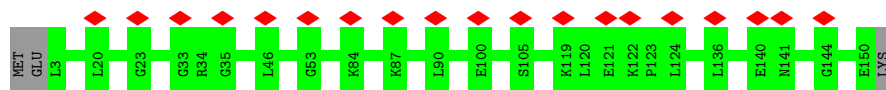


- Molecule 34: 50S ribosomal protein L14

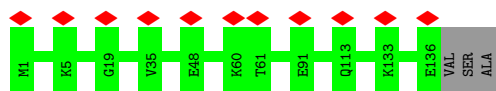


- Molecule 35: 50S ribosomal protein L15

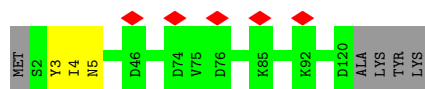




- Molecule 36: 50S ribosomal protein L16



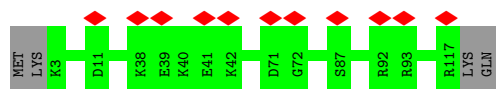
- Molecule 37: 50S ribosomal protein L17



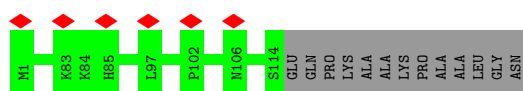
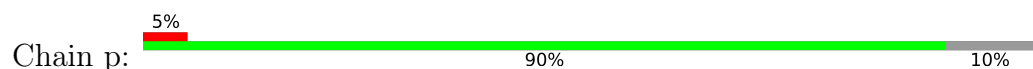
- Molecule 38: 50S ribosomal protein L18



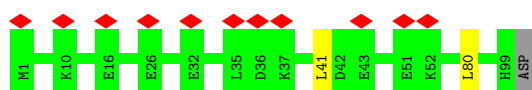
- Molecule 39: 50S ribosomal protein L19



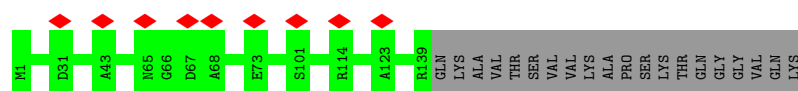
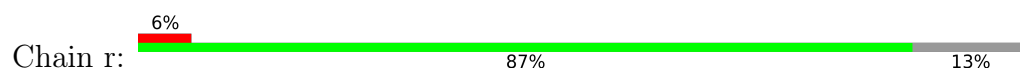
- Molecule 40: 50S ribosomal protein L20



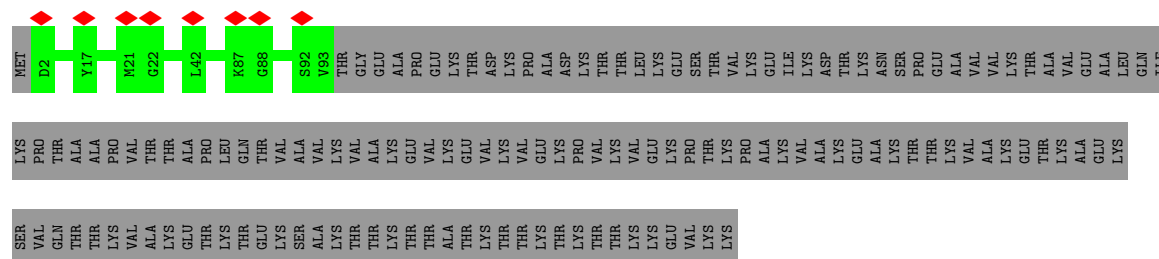
- Molecule 41: 50S ribosomal protein L21



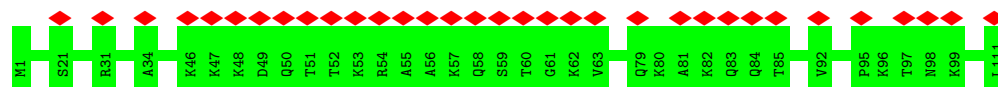
- Molecule 42: 50S ribosomal protein L22



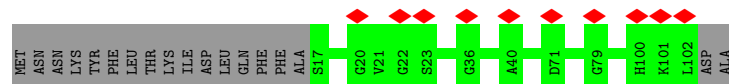
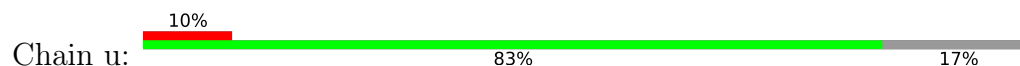
- Molecule 43: 50S ribosomal protein L23



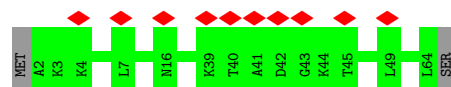
- Molecule 44: 50S ribosomal protein L24



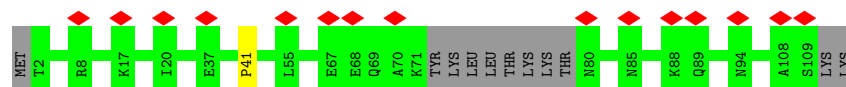
- Molecule 45: 50S ribosomal protein L27



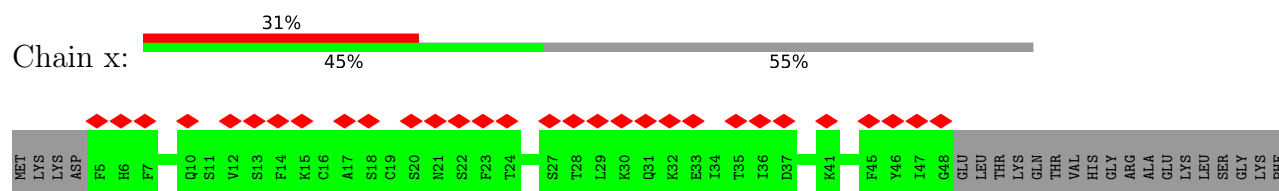
- Molecule 46: 50S ribosomal protein L28



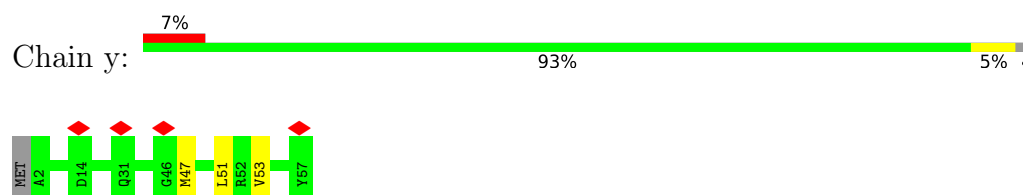
- Molecule 47: 50S ribosomal protein L29



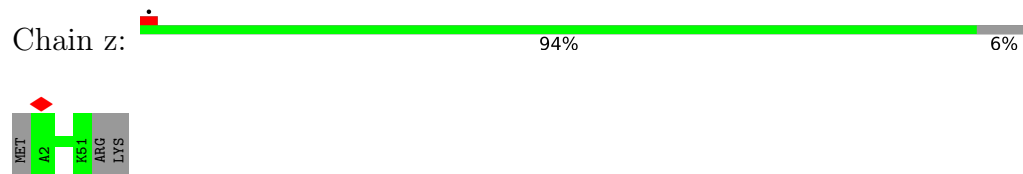
- Molecule 48: 50S ribosomal protein L31



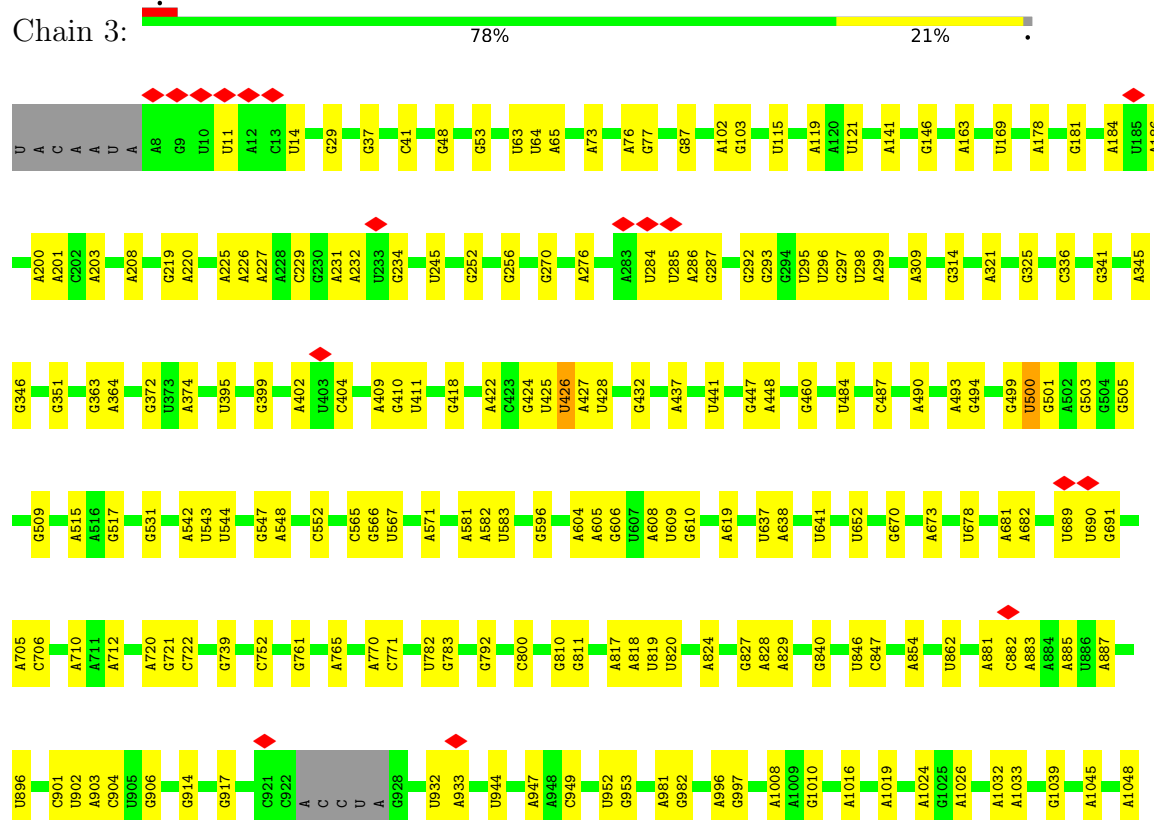
- Molecule 49: 50S ribosomal protein L32

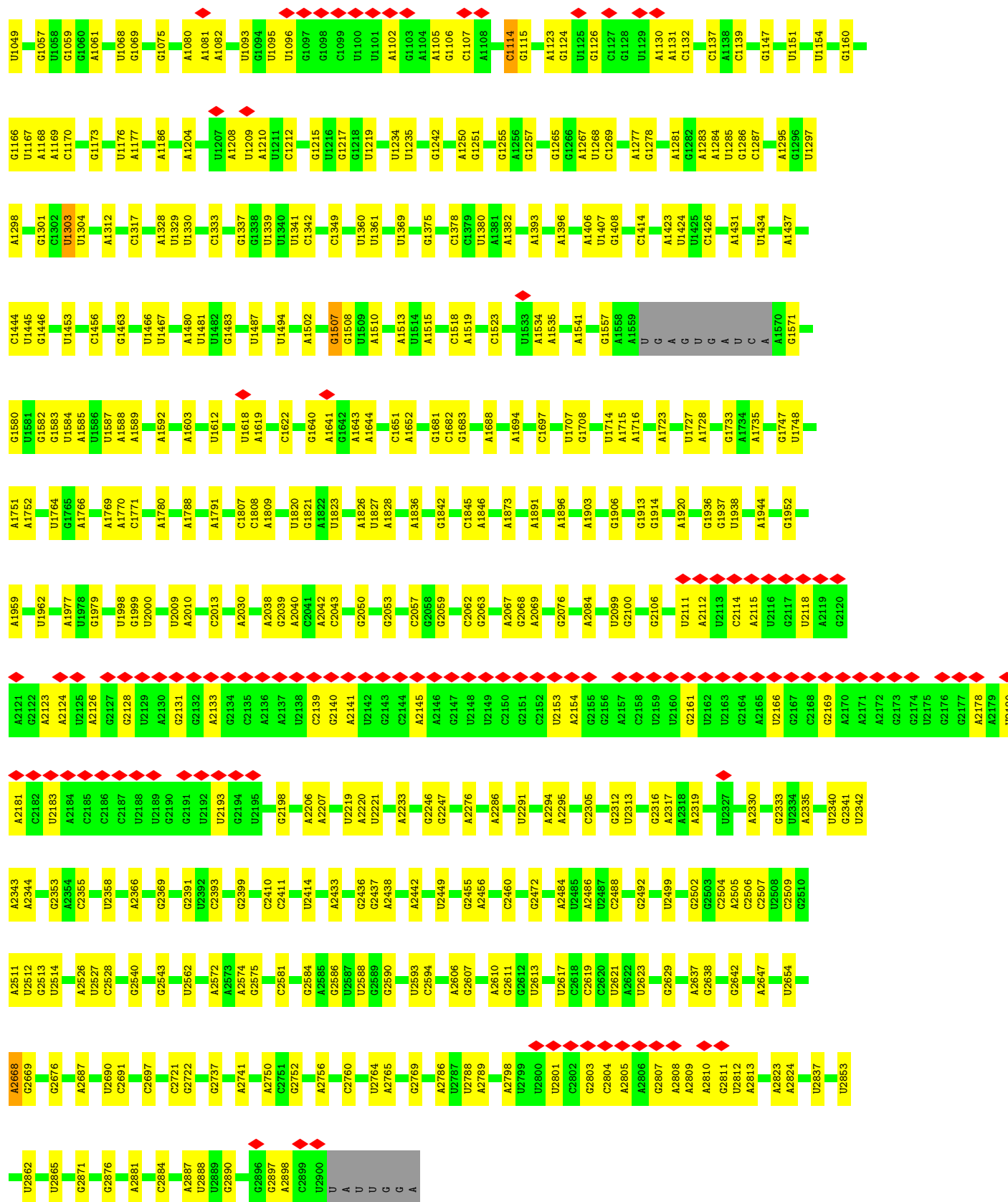



- Molecule 50: 50S ribosomal protein L33 1



- Molecule 51: 23S ribosomal RNA



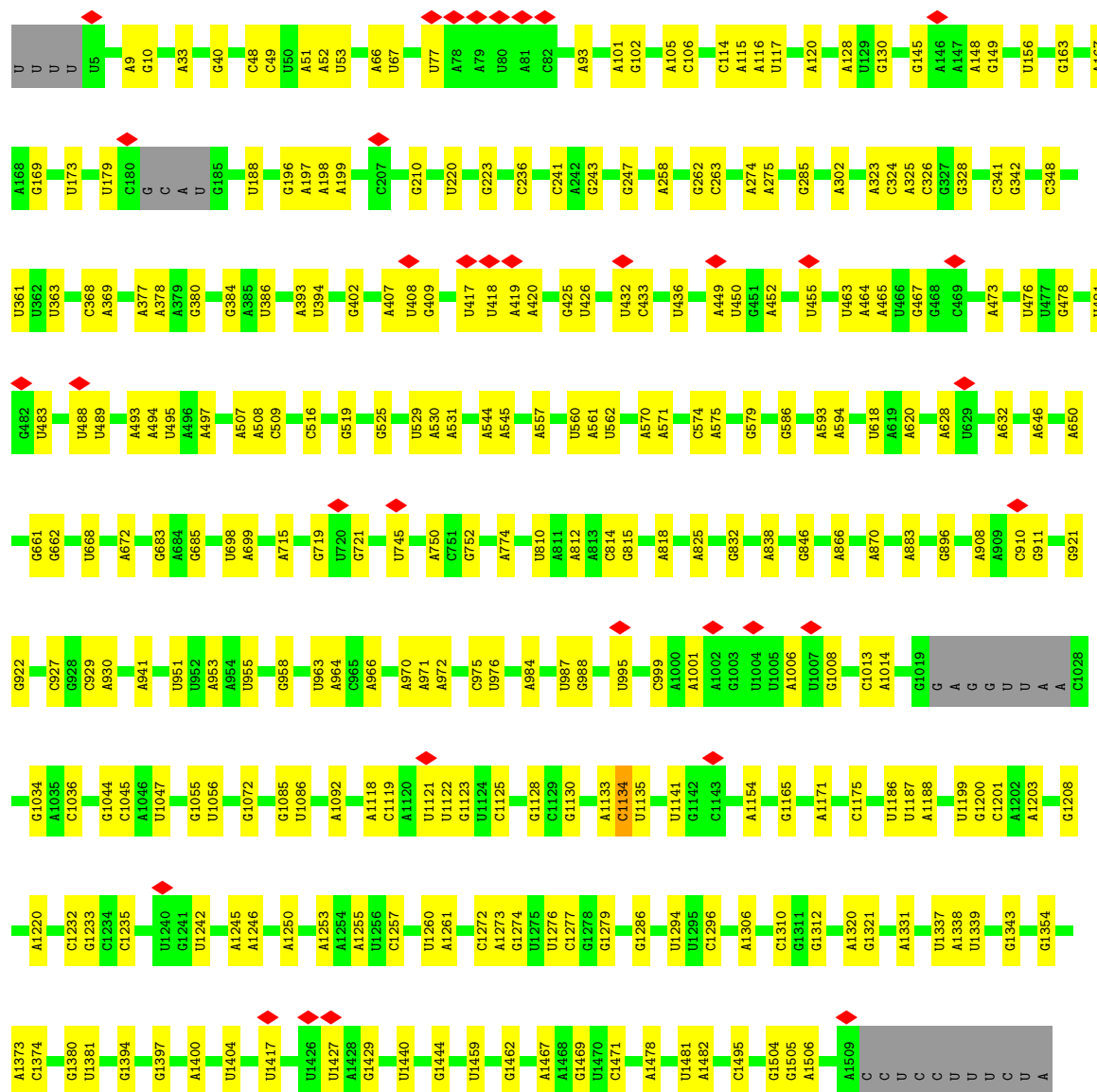


Chain 4: 



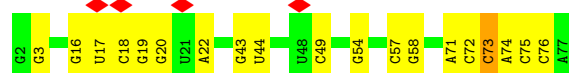
• Molecule 53: 16S ribosomal RNA

Chain 5: 



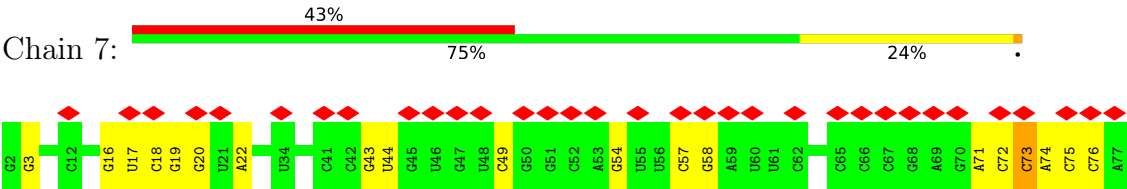
• Molecule 54: tRNA-Phe

Chain 6: 





• Molecule 54: tRNA-Phe



• Molecule 55: mRNA



There are no outlier residues recorded for this chain.

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	32086	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	3.2	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3750	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.977	Depositor
Minimum map value	-1.334	Depositor
Average map value	0.025	Depositor
Map value standard deviation	0.150	Depositor
Recommended contour level	0.65	Depositor
Map size (Å)	435.328, 435.328, 435.328	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.7005, 1.7005, 1.7005	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	0	0.23	0/383	0.46	0/504
2	1	0.23	0/484	0.48	0/637
3	2	0.23	0/306	0.47	0/401
4	A	0.26	0/1954	0.47	0/2642
5	B	0.26	0/1721	0.52	1/2323 (0.0%)
6	C	0.27	0/1691	0.47	1/2267 (0.0%)
7	D	0.24	0/1188	0.50	0/1593
8	E	0.25	0/1384	0.46	0/1867
9	F	0.27	0/1266	0.49	0/1700
10	G	0.25	0/1126	0.50	0/1517
11	H	0.25	0/1044	0.49	0/1395
12	I	0.25	0/820	0.53	0/1103
13	J	0.25	0/844	0.46	0/1136
14	K	0.27	0/1094	0.54	0/1468
15	L	0.26	0/962	0.49	0/1289
16	M	0.25	0/483	0.43	0/643
17	N	0.23	0/679	0.44	0/907
18	O	0.24	0/659	0.44	0/885
19	P	0.24	0/684	0.46	0/913
20	Q	0.25	0/545	0.46	0/730
21	R	0.27	0/698	0.48	0/936
22	S	0.24	0/631	0.46	0/838
23	T	0.26	0/475	0.43	0/621
24	Z	0.23	0/30	0.69	0/41
25	a	0.24	0/2267	0.47	1/3044 (0.0%)
26	b	0.26	0/1795	0.50	0/2412
27	c	0.25	0/1671	0.48	1/2246 (0.0%)
28	d	0.25	0/1409	0.50	1/1894 (0.1%)
29	e	0.26	0/1420	0.51	0/1912
30	f	0.24	0/1183	0.43	0/1587
31	g	0.35	0/969	0.57	0/1295
32	h	0.25	0/968	0.48	0/1298
33	i	0.28	0/1186	0.51	0/1592
34	j	0.26	0/953	0.48	0/1275

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
35	k	0.25	0/1170	0.50	0/1559
36	l	0.25	0/1104	0.48	0/1481
37	m	0.29	0/973	0.53	0/1309
38	n	0.25	0/897	0.49	0/1198
39	o	0.24	0/948	0.50	0/1262
40	p	0.27	0/961	0.49	0/1278
41	q	0.26	0/828	0.55	2/1111 (0.2%)
42	r	0.25	0/1077	0.46	0/1441
43	s	0.26	0/732	0.50	0/988
44	t	0.26	0/879	0.51	0/1165
45	u	0.25	0/665	0.48	0/884
46	v	0.23	0/519	0.46	0/695
47	w	0.26	0/826	0.48	1/1104 (0.1%)
48	x	0.26	0/353	0.47	0/474
49	y	0.30	0/457	0.56	0/601
50	z	0.24	0/412	0.51	0/547
51	3	0.19	0/69073	0.77	16/107710 (0.0%)
52	4	0.18	0/2505	0.74	0/3902
53	5	0.18	0/35768	0.75	8/55764 (0.0%)
54	6	0.20	0/1808	0.82	1/2817 (0.0%)
54	7	0.20	0/1808	0.82	1/2817 (0.0%)
55	Y	0.15	0/203	0.69	0/313
All	All	0.21	0/158938	0.70	34/237331 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
6	C	0	1
21	R	0	1
31	g	0	1
37	m	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	3	567	U	C2-N1-C1'	7.90	127.18	117.70
53	5	361	U	C2-N1-C1'	7.84	127.11	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	w	41	PRO	CA-N-CD	-7.65	100.79	111.50
51	3	567	U	N1-C2-O2	7.30	127.91	122.80
51	3	1507	G	O4'-C1'-N9	6.77	113.62	108.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	C	1	MET	Peptide
21	R	25	GLN	Peptide
31	g	114	ASP	Peptide
37	m	3	TYR	Peptide

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	45/48 (94%)	43 (96%)	2 (4%)	0	100	100
2	1	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
3	2	35/37 (95%)	35 (100%)	0	0	100	100
4	A	238/294 (81%)	214 (90%)	24 (10%)	0	100	100
5	B	213/273 (78%)	196 (92%)	17 (8%)	0	100	100
6	C	201/205 (98%)	187 (93%)	14 (7%)	0	100	100
7	D	151/219 (69%)	145 (96%)	6 (4%)	0	100	100
8	E	165/215 (77%)	144 (87%)	21 (13%)	0	100	100
9	F	152/155 (98%)	143 (94%)	9 (6%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	G	139/142 (98%)	126 (91%)	13 (9%)	0	100	100
11	H	126/132 (96%)	111 (88%)	15 (12%)	0	100	100
12	I	99/108 (92%)	89 (90%)	10 (10%)	0	100	100
13	J	112/121 (93%)	110 (98%)	2 (2%)	0	100	100
14	K	134/139 (96%)	119 (89%)	15 (11%)	0	100	100
15	L	116/124 (94%)	104 (90%)	12 (10%)	0	100	100
16	M	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
17	N	81/86 (94%)	78 (96%)	3 (4%)	0	100	100
18	O	78/94 (83%)	72 (92%)	6 (8%)	0	100	100
19	P	81/85 (95%)	75 (93%)	6 (7%)	0	100	100
20	Q	63/104 (61%)	55 (87%)	8 (13%)	0	100	100
21	R	82/87 (94%)	70 (85%)	12 (15%)	0	100	100
22	S	75/87 (86%)	73 (97%)	2 (3%)	0	100	100
23	T	51/60 (85%)	49 (96%)	2 (4%)	0	100	100
24	Z	3/5 (60%)	2 (67%)	1 (33%)	0	100	100
25	a	283/287 (99%)	264 (93%)	19 (7%)	0	100	100
26	b	227/287 (79%)	216 (95%)	11 (5%)	0	100	100
27	c	208/212 (98%)	198 (95%)	10 (5%)	0	100	100
28	d	173/180 (96%)	157 (91%)	16 (9%)	0	100	100
29	e	174/184 (95%)	161 (92%)	13 (8%)	0	100	100
30	f	143/149 (96%)	131 (92%)	12 (8%)	0	100	100
31	g	124/161 (77%)	112 (90%)	11 (9%)	1 (1%)	16	54
32	h	126/137 (92%)	121 (96%)	5 (4%)	0	100	100
33	i	142/146 (97%)	135 (95%)	7 (5%)	0	100	100
34	j	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
35	k	146/151 (97%)	134 (92%)	12 (8%)	0	100	100
36	l	134/139 (96%)	130 (97%)	4 (3%)	0	100	100
37	m	117/124 (94%)	109 (93%)	7 (6%)	1 (1%)	14	51
38	n	108/116 (93%)	100 (93%)	8 (7%)	0	100	100
39	o	113/119 (95%)	104 (92%)	9 (8%)	0	100	100
40	p	112/127 (88%)	107 (96%)	5 (4%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	q	97/100 (97%)	90 (93%)	7 (7%)	0	100	100
42	r	137/159 (86%)	127 (93%)	10 (7%)	0	100	100
43	s	90/237 (38%)	84 (93%)	6 (7%)	0	100	100
44	t	109/111 (98%)	104 (95%)	5 (5%)	0	100	100
45	u	84/104 (81%)	80 (95%)	4 (5%)	0	100	100
46	v	61/65 (94%)	57 (93%)	4 (7%)	0	100	100
47	w	96/111 (86%)	92 (96%)	4 (4%)	0	100	100
48	x	42/97 (43%)	34 (81%)	8 (19%)	0	100	100
49	y	54/57 (95%)	49 (91%)	4 (7%)	1 (2%)	6	32
50	z	48/53 (91%)	47 (98%)	1 (2%)	0	100	100
All	All	5823/6675 (87%)	5407 (93%)	413 (7%)	3 (0%)	50	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
37	m	4	ILE
49	y	53	VAL
31	g	87	ASN

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	40/41 (98%)	40 (100%)	0	100	100
2	1	51/51 (100%)	51 (100%)	0	100	100
3	2	35/35 (100%)	35 (100%)	0	100	100
4	A	212/262 (81%)	212 (100%)	0	100	100
5	B	180/232 (78%)	179 (99%)	1 (1%)	84	88
6	C	181/183 (99%)	179 (99%)	2 (1%)	70	80
7	D	123/178 (69%)	122 (99%)	1 (1%)	79	85

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	E	150/196 (76%)	150 (100%)	0	100	100
9	F	131/132 (99%)	131 (100%)	0	100	100
10	G	123/124 (99%)	123 (100%)	0	100	100
11	H	111/115 (96%)	110 (99%)	1 (1%)	75	83
12	I	95/99 (96%)	95 (100%)	0	100	100
13	J	91/97 (94%)	91 (100%)	0	100	100
14	K	117/120 (98%)	115 (98%)	2 (2%)	56	73
15	L	100/105 (95%)	100 (100%)	0	100	100
16	M	47/48 (98%)	47 (100%)	0	100	100
17	N	76/78 (97%)	76 (100%)	0	100	100
18	O	69/82 (84%)	67 (97%)	2 (3%)	37	58
19	P	73/75 (97%)	73 (100%)	0	100	100
20	Q	56/94 (60%)	56 (100%)	0	100	100
21	R	74/77 (96%)	74 (100%)	0	100	100
22	S	70/77 (91%)	67 (96%)	3 (4%)	25	47
23	T	49/56 (88%)	49 (100%)	0	100	100
24	Z	3/3 (100%)	3 (100%)	0	100	100
25	a	241/243 (99%)	241 (100%)	0	100	100
26	b	186/233 (80%)	186 (100%)	0	100	100
27	c	182/184 (99%)	182 (100%)	0	100	100
28	d	150/154 (97%)	149 (99%)	1 (1%)	81	87
29	e	153/159 (96%)	151 (99%)	2 (1%)	65	77
30	f	123/134 (92%)	121 (98%)	2 (2%)	58	75
31	g	101/129 (78%)	90 (89%)	11 (11%)	5	19
32	h	102/110 (93%)	101 (99%)	1 (1%)	73	82
33	i	126/128 (98%)	125 (99%)	1 (1%)	79	85
34	j	103/103 (100%)	103 (100%)	0	100	100
35	k	123/126 (98%)	123 (100%)	0	100	100
36	l	113/115 (98%)	113 (100%)	0	100	100
37	m	105/109 (96%)	104 (99%)	1 (1%)	73	82
38	n	96/99 (97%)	94 (98%)	2 (2%)	48	67

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	o	101/105 (96%)	101 (100%)	0	100	100
40	p	100/108 (93%)	100 (100%)	0	100	100
41	q	90/91 (99%)	90 (100%)	0	100	100
42	r	116/132 (88%)	116 (100%)	0	100	100
43	s	82/208 (39%)	82 (100%)	0	100	100
44	t	96/96 (100%)	96 (100%)	0	100	100
45	u	69/85 (81%)	69 (100%)	0	100	100
46	v	58/60 (97%)	58 (100%)	0	100	100
47	w	87/98 (89%)	87 (100%)	0	100	100
48	x	41/86 (48%)	41 (100%)	0	100	100
49	y	48/49 (98%)	46 (96%)	2 (4%)	25	47
50	z	47/50 (94%)	47 (100%)	0	100	100
All	All	5096/5754 (89%)	5061 (99%)	35 (1%)	80	87

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	h	95	LYS
33	i	64	GLN
38	n	63	LYS
28	d	27	GLN
22	S	63	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
35	k	36	GLN
40	p	36	GLN
42	r	38	ASN
41	q	87	GLN
36	l	99	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
51	3	2875/2907 (98%)	587 (20%)	25 (0%)

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
52	4	103/108 (95%)	24 (23%)	2 (1%)
53	5	1490/1520 (98%)	279 (18%)	5 (0%)
54	6	75/76 (98%)	18 (24%)	1 (1%)
54	7	75/76 (98%)	18 (24%)	1 (1%)
55	Y	8/9 (88%)	0	0
All	All	4626/4696 (98%)	926 (20%)	34 (0%)

5 of 926 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
51	3	11	U
51	3	29	G
51	3	37	G
51	3	41	C
51	3	48	G

5 of 34 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
53	5	419	A
53	5	1186	U
54	6	16	G
51	3	1507	G
51	3	1297	U

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

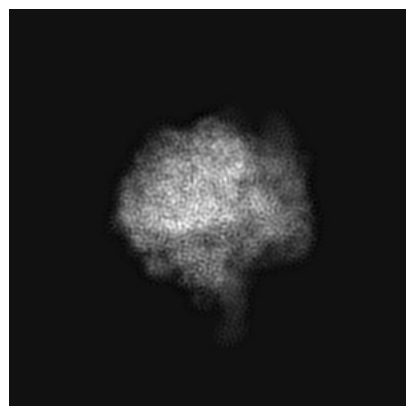
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13276. These allow visual inspection of the internal detail of the map and identification of artifacts.

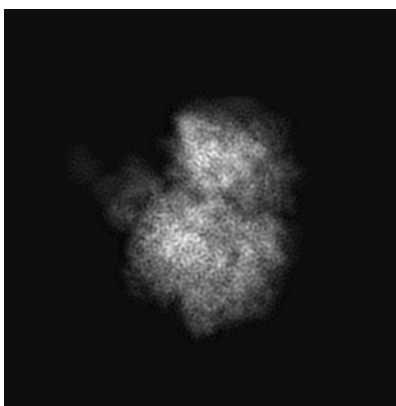
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

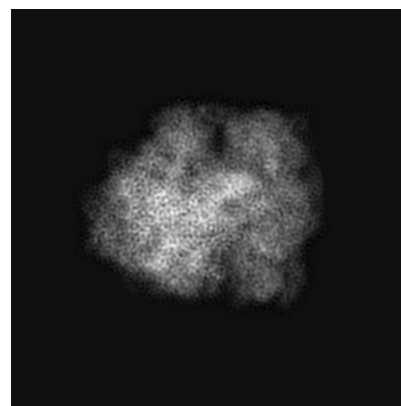
#### 6.1.1 Primary map



X

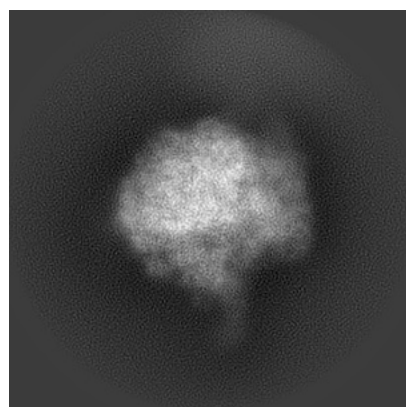


Y

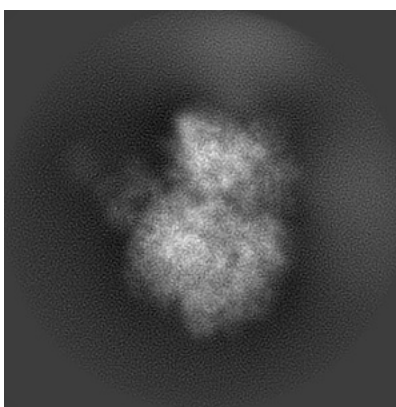


Z

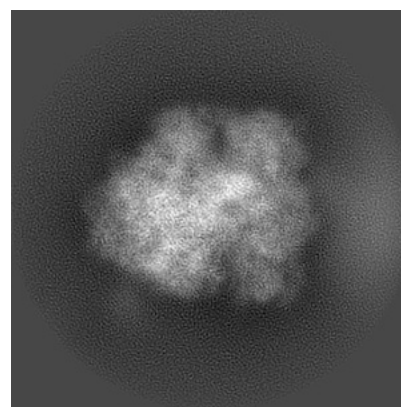
#### 6.1.2 Raw map



X



Y

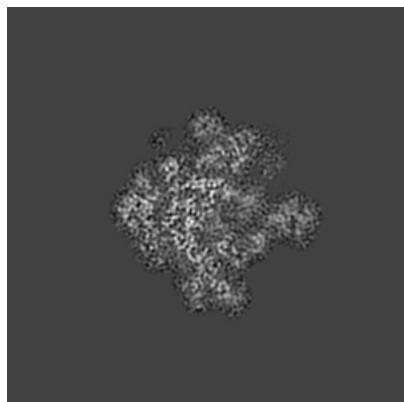


Z

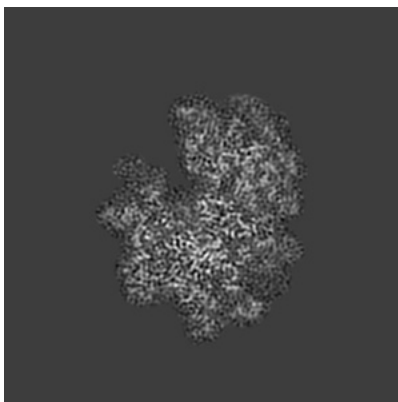
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

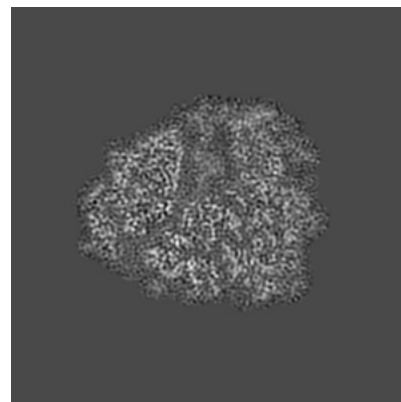
### 6.2.1 Primary map



X Index: 128

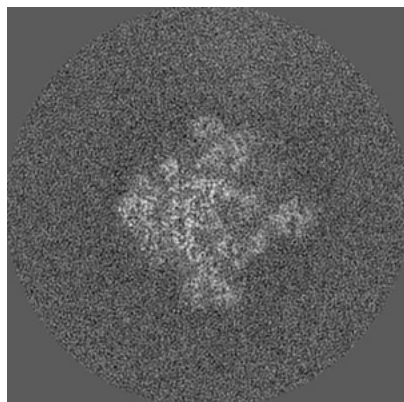


Y Index: 128

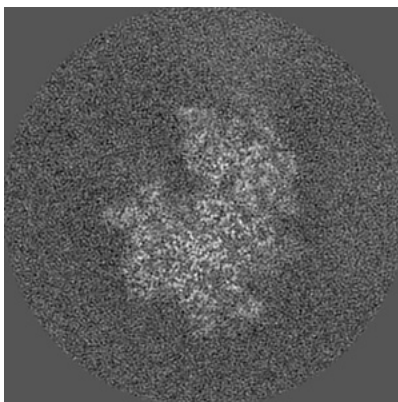


Z Index: 128

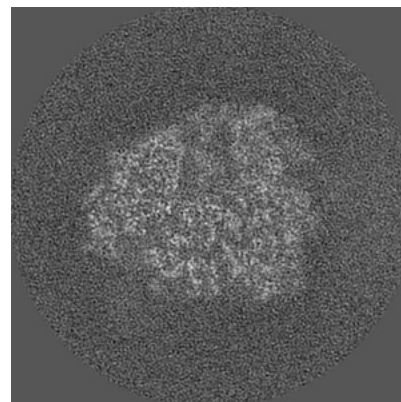
### 6.2.2 Raw map



X Index: 128



Y Index: 128

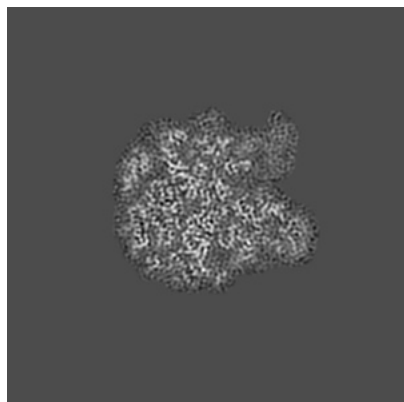


Z Index: 128

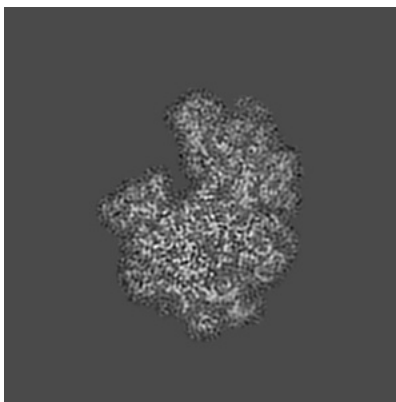
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

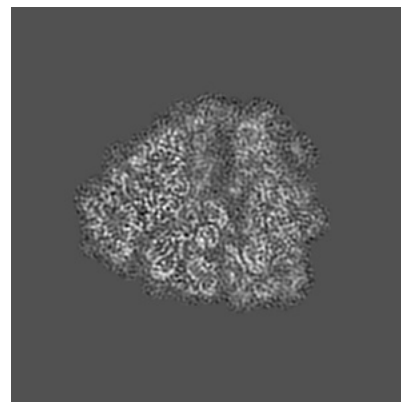
### 6.3.1 Primary map



X Index: 103

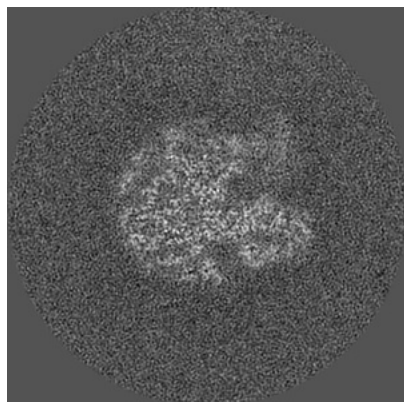


Y Index: 122

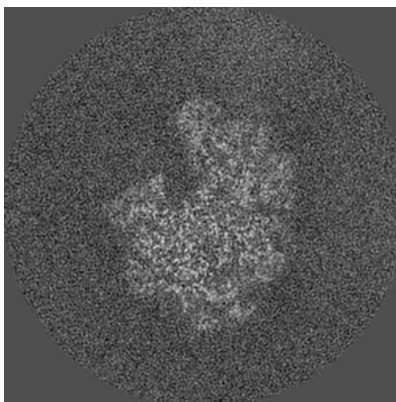


Z Index: 125

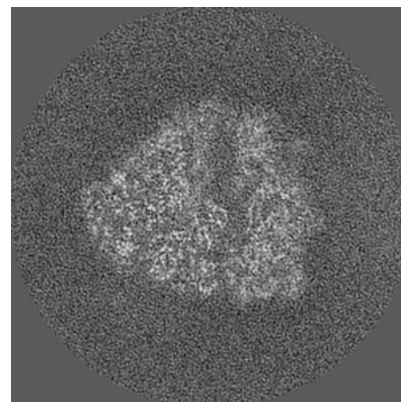
### 6.3.2 Raw map



X Index: 108



Y Index: 122



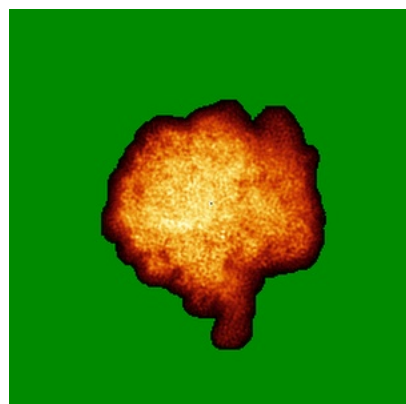
Z Index: 124

The images above show the largest variance slices of the map in three orthogonal directions.

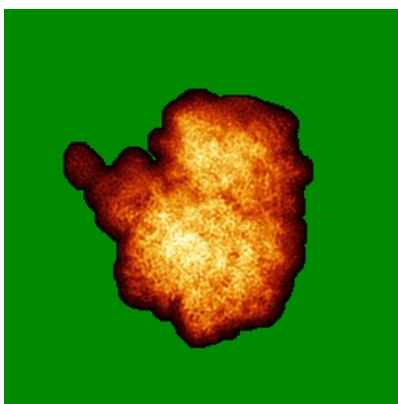


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

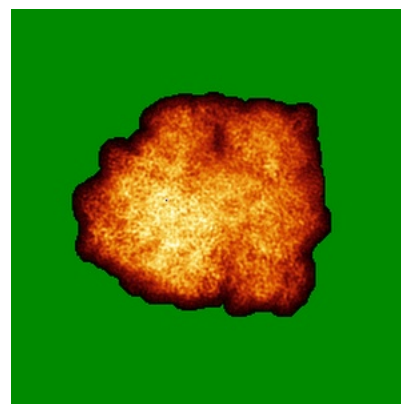
### 6.4.1 Primary map



X

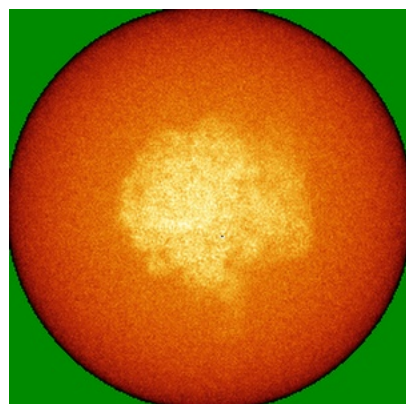


Y

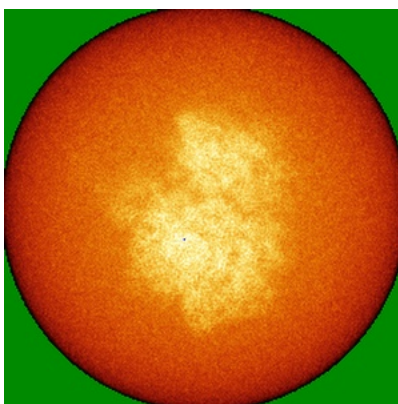


Z

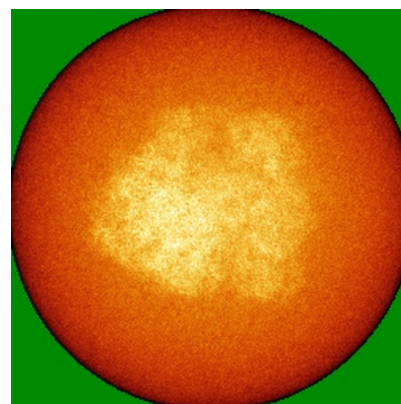
### 6.4.2 Raw map



X



Y

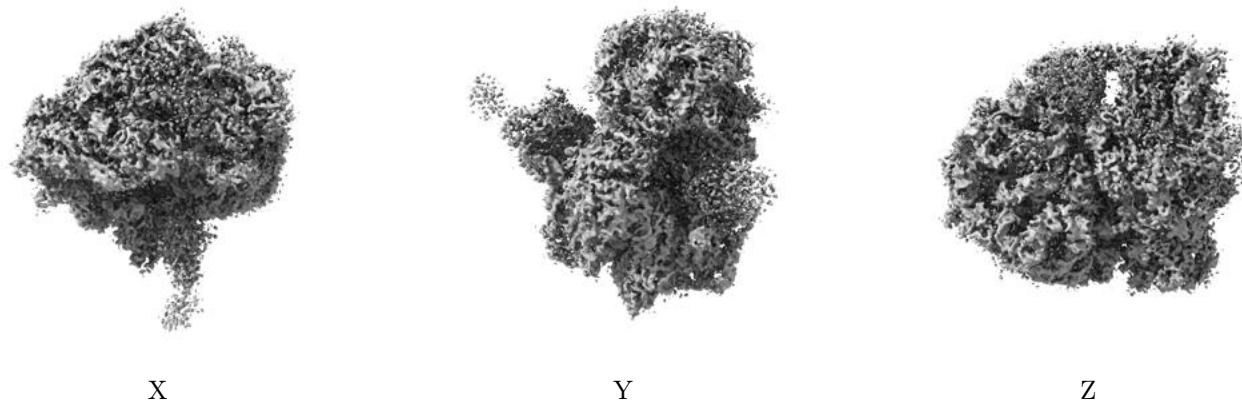


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

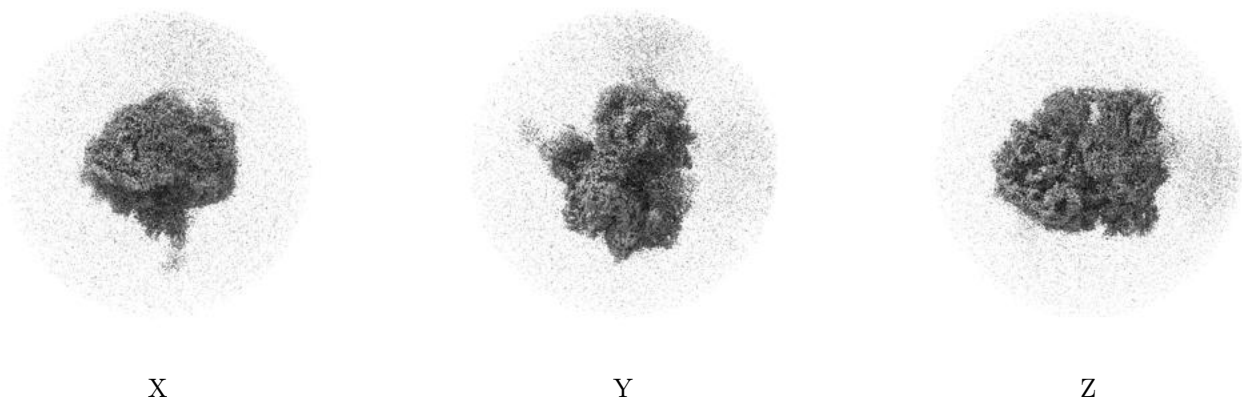
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.65. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.



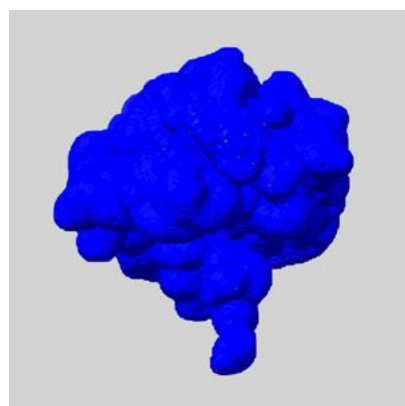
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

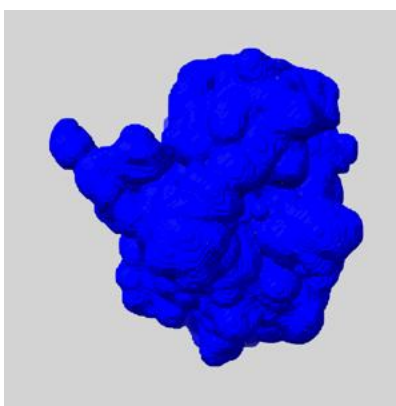
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

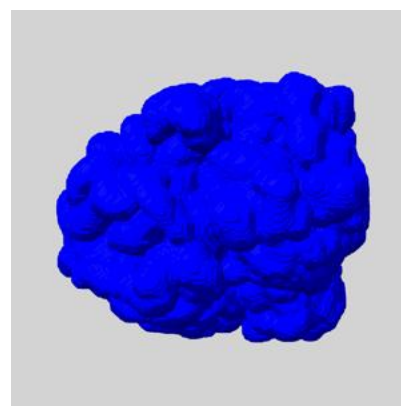
### 6.6.1 emd\_13276\_msk\_1.map [i](#)



X



Y

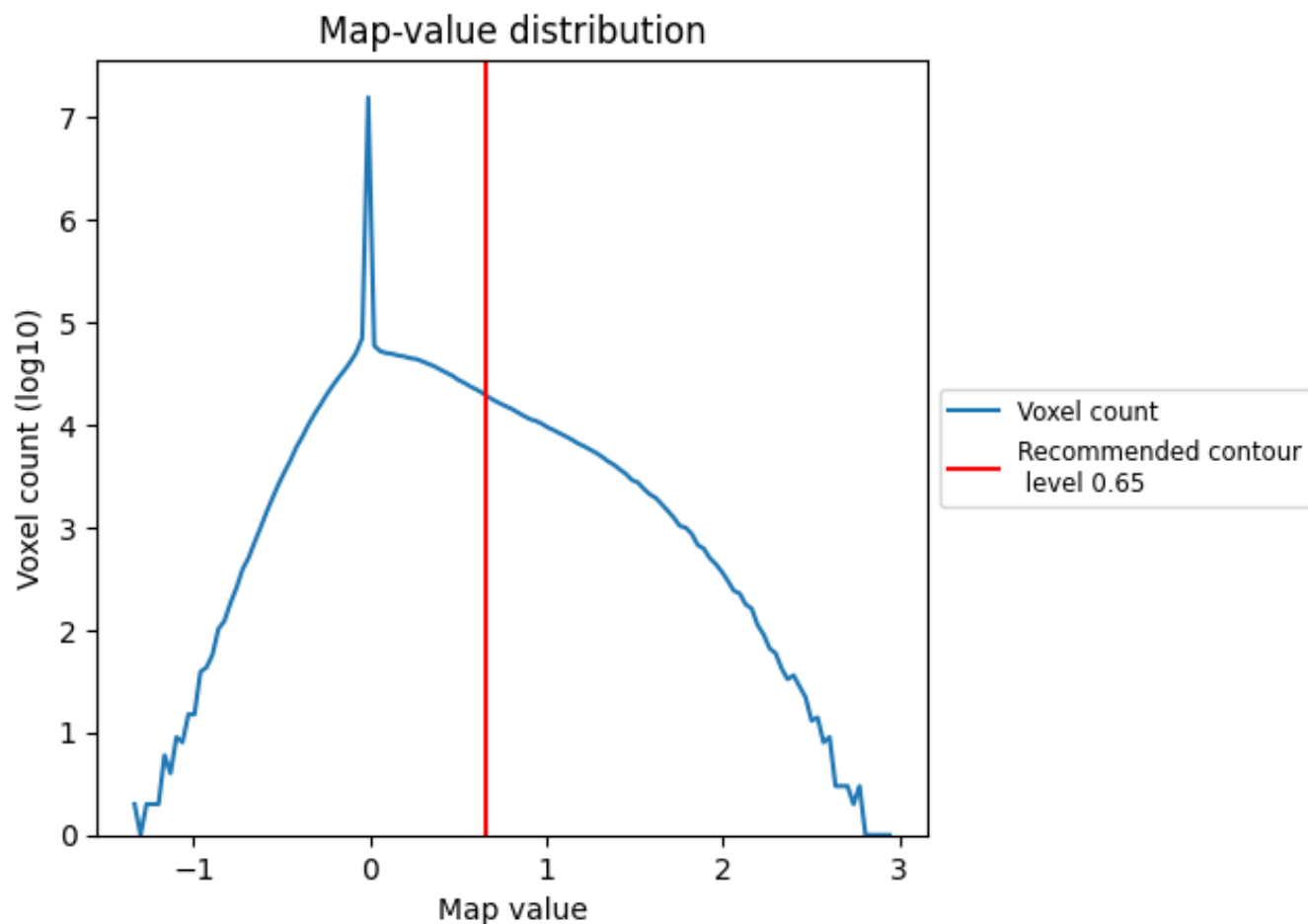


Z

## 7 Map analysis [i](#)

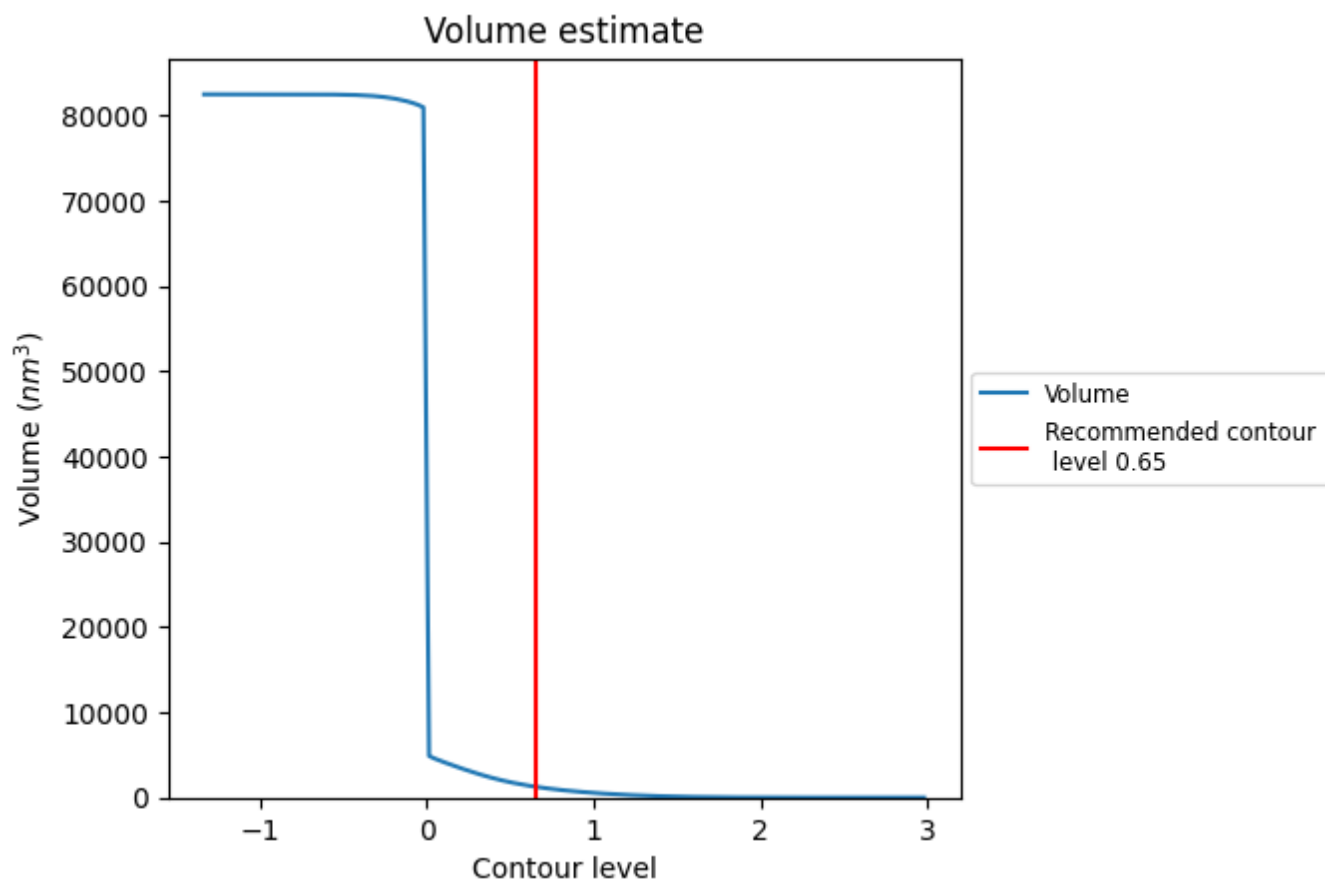
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

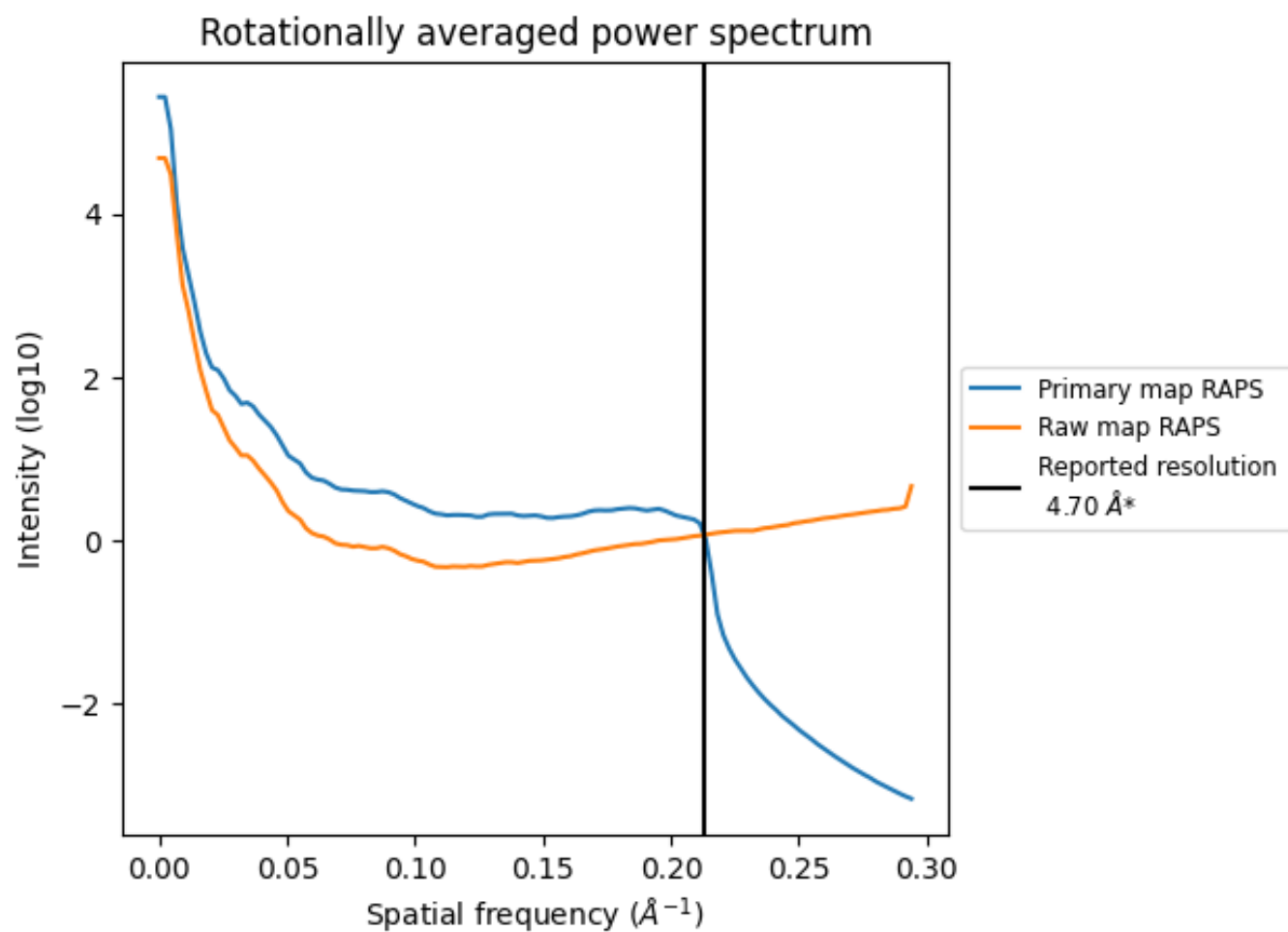
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1271  $\text{nm}^3$ ; this corresponds to an approximate mass of 1148 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

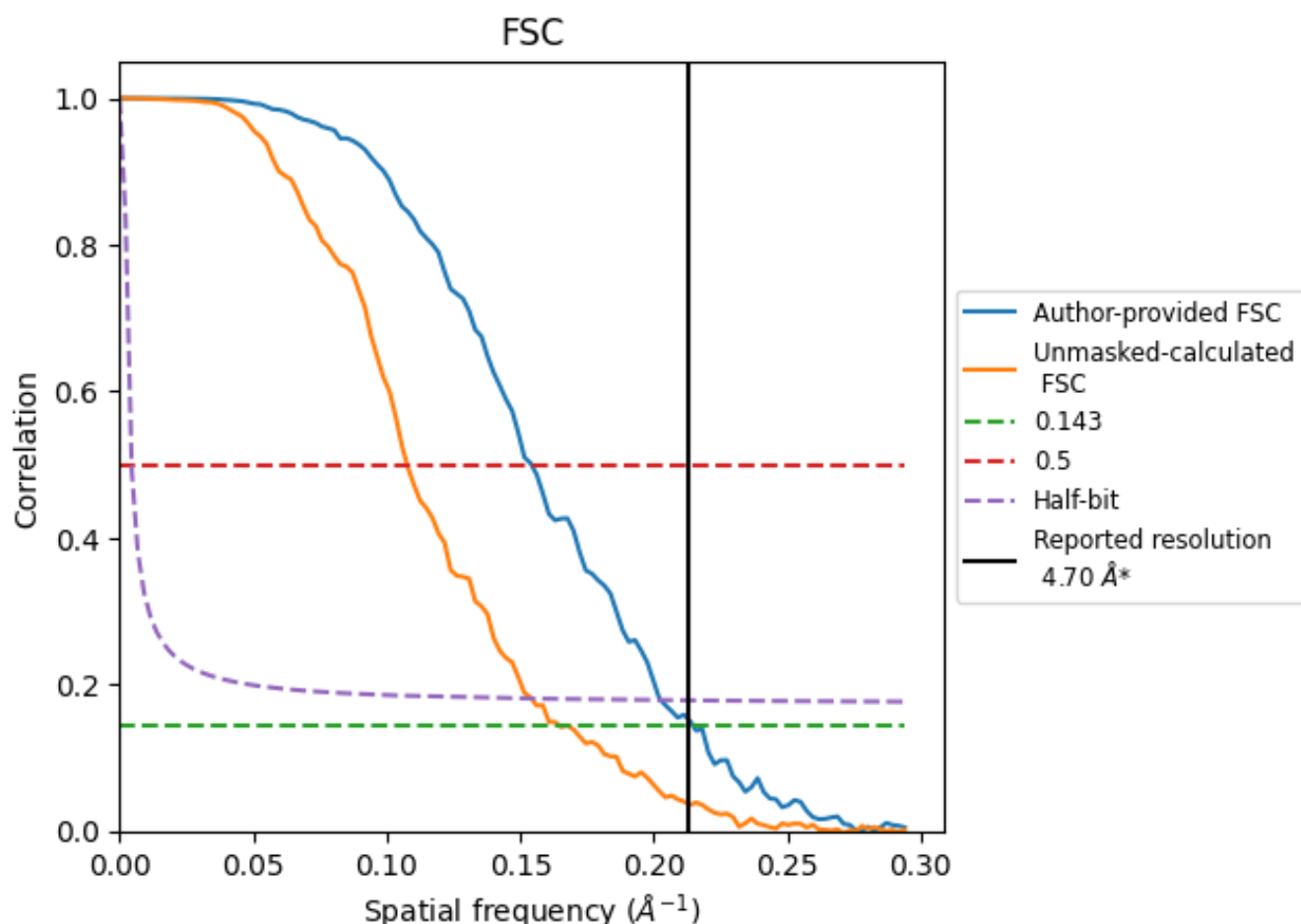


\*Reported resolution corresponds to spatial frequency of  $0.213 \text{ \AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.213 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

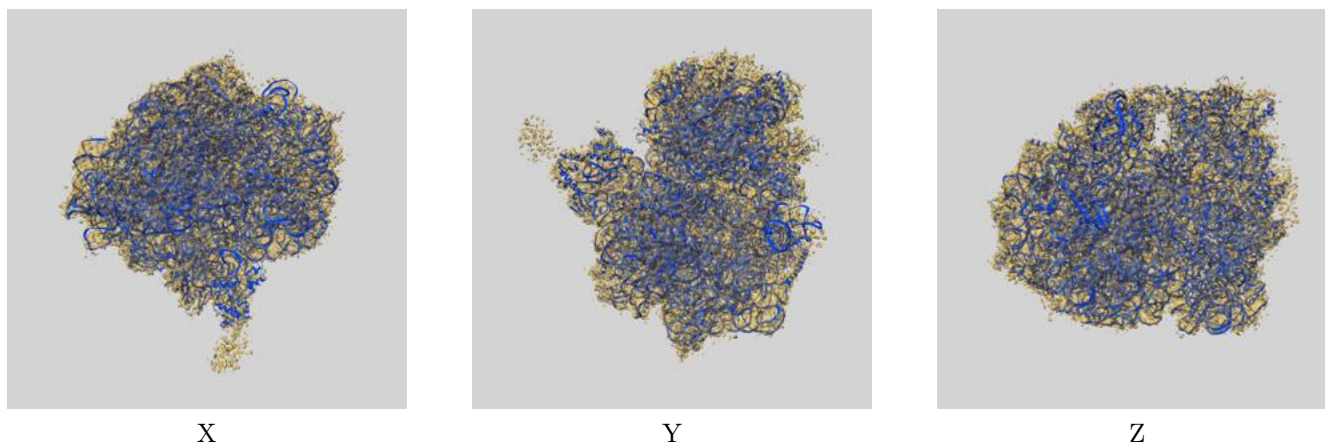
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	4.66	6.49	4.93
Unmasked-calculated*	6.06	9.29	6.48

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.06 differs from the reported value 4.7 by more than 10 %

## 9 Map-model fit [i](#)

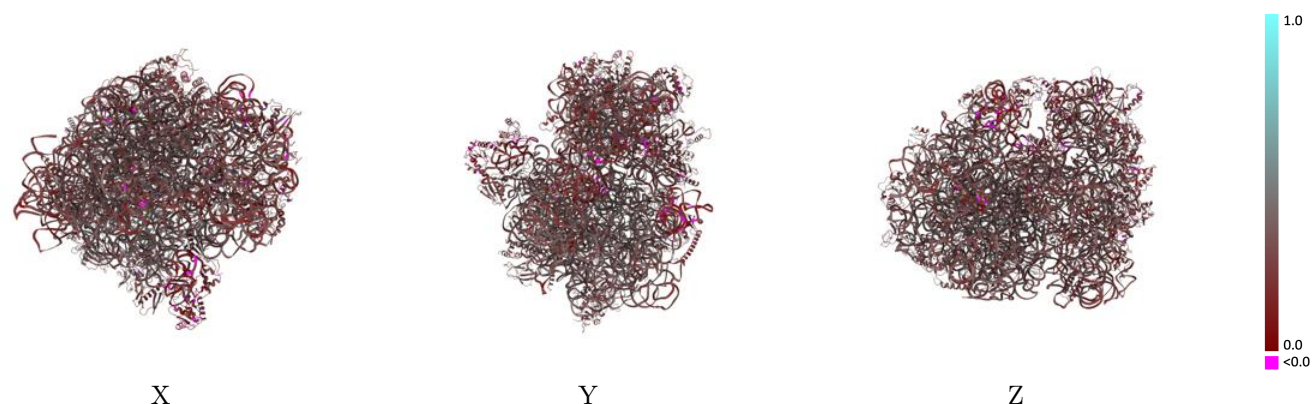
This section contains information regarding the fit between EMDB map EMD-13276 and PDB model 7PAL. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

### 9.1 Map-model overlay [i](#)



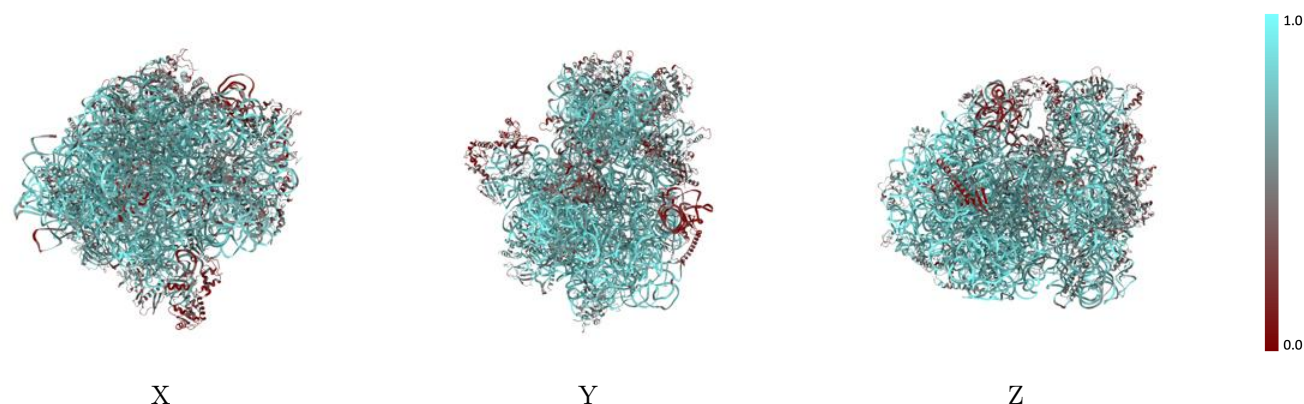
The images above show the 3D surface view of the map at the recommended contour level 0.65 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

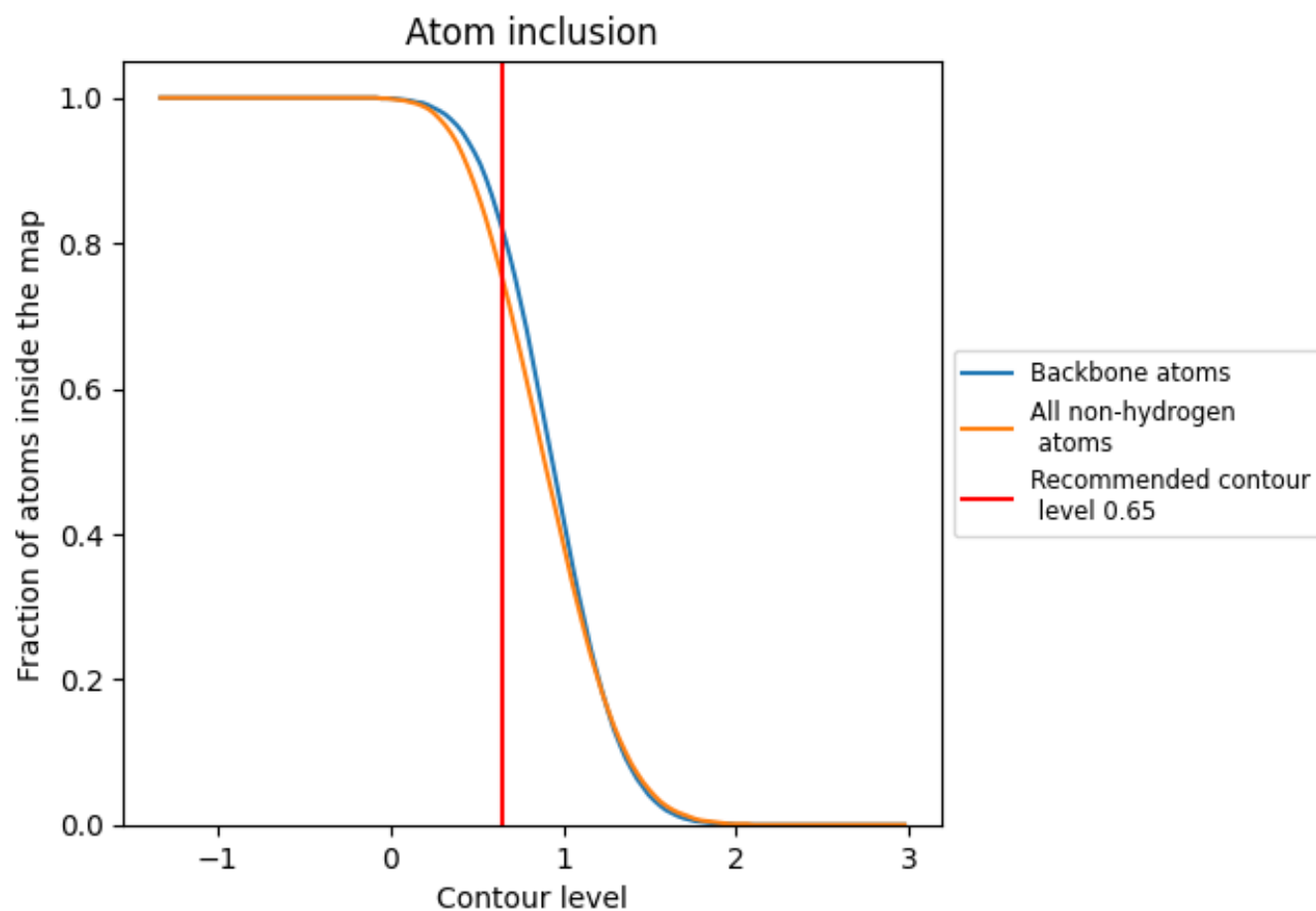
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.65).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ













































The table lists the average atom inclusion at the recommended contour level (0.65) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7490	 0.3240
0	 0.7810	 0.3900
1	 0.7210	 0.3840
2	 0.7570	 0.3980
3	 0.8500	 0.3360
4	 0.8490	 0.3230
5	 0.8350	 0.3140
6	 0.7460	 0.2760
7	 0.4730	 0.1370
A	 0.4840	 0.2990
B	 0.5330	 0.3190
C	 0.5170	 0.2990
D	 0.5850	 0.3400
E	 0.4360	 0.3010
F	 0.4250	 0.2600
G	 0.5520	 0.3180
H	 0.4800	 0.2820
I	 0.5030	 0.3110
J	 0.5500	 0.3210
K	 0.6310	 0.3660
L	 0.3930	 0.2640
M	 0.6260	 0.3170
N	 0.5260	 0.2950
O	 0.5800	 0.3300
P	 0.5450	 0.3290
Q	 0.5430	 0.3020
R	 0.4550	 0.2820
S	 0.5820	 0.2880
T	 0.5220	 0.3260
Y	 0.8740	 0.3590
Z	 0.6770	 0.3370
a	 0.6940	 0.3750
b	 0.6780	 0.3660
c	 0.6310	 0.3570
d	 0.4230	 0.2450



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
e	 0.5340	 0.3210
f	 0.1870	 0.2380
g	 0.2460	 0.1980
h	 0.1330	 0.2190
i	 0.6580	 0.3570
j	 0.6510	 0.3830
k	 0.6730	 0.3660
l	 0.6870	 0.3700
m	 0.6860	 0.3480
n	 0.5960	 0.3230
o	 0.6440	 0.3610
p	 0.6940	 0.3200
q	 0.6520	 0.3790
r	 0.7230	 0.3710
s	 0.6600	 0.3730
t	 0.5120	 0.3540
u	 0.6780	 0.3620
v	 0.6830	 0.3710
w	 0.5870	 0.3380
x	 0.3410	 0.2780
y	 0.6750	 0.3620
z	 0.7080	 0.3670